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July 24, 2003

Ms. Marianne L. Horinko Acting Administrator U.S. Environmental Protection Agency P.O. Box 1473 Merrifield, VA 22116 Attn: Chemical Right-to-Know Program

Re: HPV Challenge Program, AR-201

Terphenyl, Mixed; CAS Number 26140-60-3 Quaterphenyl; CAS Number 29036-02-0

Solutia, Inc., Company Registration Number is pleased to submit the attached Test Plan and Robust Summaries for the Category Polyphenyls (Mixed Terphenyls, CAS Number 26140-60-3 and Quaterphenyls, CAS Number 29036-02-0) as a part of our commitment to the EPA High Production Volume Challenge Program, AR-201. Although not part of the category, we have also included information on ortho-Terphenyl, CAS Number 84-15-1; m-Terphenyl, CAS Number 92-06-8; and p-Terphenyl; CAS Number 92-94-4 to support our data.

The attached files are:

- 1. This cover letter in MS Word 2000
- 2. Test Plan in MS Word 2000
- 3. Robust Summaries (IUCLID format) in MS Word 2000

The complete matrix of SIDS data elements, including physical/chemical properties and results of biological and toxicology studies, indicate the need for additional testing.

Please contact me at 314-674-1113 if there are any questions relating to this submission.

Regards,

Donald A. Lederer Product Stewardship Manager

# HIGH PRODUCTION VOLUME (HPV) CHEMICAL CHALLENGE PROGRAM

## **TEST PLAN**

## For the

## POLYPHENYL (3- & 4-PHENYL RINGS) CATEGORY

CAS Number 26140-60-3; Terphenyls, Mixed

CAS Number 29036-02-0; Quaterphenyls

## Prepared by:

Solutia Inc. Registration No.

575 Maryville Centre Drive, St. Louis, Missouri 63141

July 23, 2003

## **EXECUTIVE SUMMARY**

Solutia Inc. voluntarily submits the following Category Justification, Screening Information Data (Robust Summaries) and Test Plan for review under the Environmental Protection Agency's High Production Volume (HPV) Chemicals Challenge Program. The Category, entitled "Polyphenyls (3- & 4-Phenyl Rings)" consists of two members, Terphenyls, Mixed (CAS No. 26140-60-3), and Quaterphenyls (CAS No. 29036-02-0), each consisting of multiple isomers. This Category is justified on the basis of chemical structure similarity, as well as similarity of basic screening data, as provided in an initial assessment of physico-chemical properties, environmental fate and human and environmental effects.

A substantial amount of data exists to evaluate the potential hazards associated with this Category of chemicals. Use of key studies available from data already developed, derived from recommended estimation models, or use of "read-across" methods collectively provide adequate support to characterize most Endpoints in the HPV Chemicals Challenge Program. Some additional testing is recommended to complete the assessment of members within this Category.

## TABLE OF CONTENTS

		Pg.
I.	INTRODUCTION AND IDENTIFICATION OF THE	
	CHEMICAL	4
	A. Structure and Nomenclature	5
	B. Manufacturing and Use	7
II.	CATEGORY JUSTIFICATION	8
III.	TEST PLAN RATIONALE	9
IV.	TEST PLAN SUMMARIES AND CONCLUSIONS	10
	A. Test Plan Testing Matrix for Terphenyls, Mixed	. 12
	B. Test Plan Testing Matrix for Quaterphenyls	
V.	DATA SET SUMMARIES AND EVALUATION	14
	A. Chemical/Physical Properties	14
	B. Environmental Fate and Biodegradation	16
	C. Aquatic Toxicity	20
	D. Mammalian Toxicity	22
	D.1 Acute Toxicity	22
	D.2 Repeated Dose Toxicity	24
	D.3 Mutagenicity and Chromosomal Aberrations	24
	D.4 Reproductive and Developmental Toxicity	26
VI	I. REFERENCES	26
VI	II. ROBUST SUMMARIES	.27

## TEST PLAN FOR POLYPHENYLS (3- & 4-Phenyl Rings)

## I. INTRODUCTION AND IDENTIFICATION OF CATEGORY MEMBERS

Under EPA's High Production Volume (HPV) Chemicals Challenge Program, Solutia Inc. has committed to voluntarily compile basic screening data on two members from the same structural family of aromatic hydrocarbons, namely Terphenyls, Mixed (CAS no. 26140-60-3) and Quaterphenyls (CAS no. 29036-02-0). Solutia Inc. believes that a Category of Polyphenyls (3- & 4-Phenyl Rings) is appropriate for this review and is scientifically justifiable. While the HPV process is based on specific chemicals as identified by CAS number, the members nominated for this Category are, in actuality, mixtures of 3- and 4-phenyl ring structures, respectfully. Further, the products tested for each Category member contain some 3-ring moieties and some 4-ring components; however, each product test article is predominated by isomeric forms synonymous with their chemical name, i.e. Terphenyls, Mixed contains a preponderance of m-terphenyl, p-terphenyl and o-terphenyl isomers with small amounts of quaterphenyls while Quaterphenyls contains a high percentage of 4-phenyl ring quaterphenyls with small amounts of 3-ring terphenyls.

The data included in this Category involve physicochemical properties, environmental fate, and human and environmental effects of the two members for which Solutia has volunteered in this Category, as defined by the Organization for Economic Cooperation and Development (OECD). However, as each member is a mixture we have also provided available data on the major components (ortho-, meta- and para-) of Mixed Terphenyl isomers as surrogates in our data assessment program. No information has been located on isolated Quaterphenyl isomers. Individual Robust Summaries have been assembled for each referenced Terphenyl component, as well as each of the two Category members nominated.

The information provided comes from existing data found in the scientific literature or developed on behalf of Solutia Inc., or its predecessor Monsanto Co. or from recommended estimation models. This submission fulfills Solutia's initial obligation to the HPV Challenge Program for these two chemicals.

## A. Structure and Nomenclature

The members of this family of Polyphenyls (3- & 4-phenyl rings) include the following chemicals:

D1 Ph

a. Terphenyls, Mixed-

CAS No. 26140-60-3

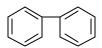
CA Index Name: Terphenyl (8CI, 9CI)

Synonyms: Benzene, diphenyl-; Benzene, [biphenyl]yl-;

Diphenylbenzene; Terbenzene; Triphenyl; Santowax R; Therminol 88;

Santowax CST; Therminol 75; MCS-1980; Santowax MP; Santowax OM;

CP 75052



2 ( D1 Ph )

b. Quaterphenyls

CAS No. 29036-02-0

CA Index Name: Quaterphenyl (7CI, 9CI)

Synonyms: Quaterbenzene; Santotar 9; Santowax Q

The following Surrogate Chemicals have been used as an aid in this assessment to evaluate the Mixed Terphenyl group, as they are primary components of that substance.

c. ortho-Terphenyl

CAS No. 100-00-5

CA Index Name: 1,1':2',1"-Terphenyl (9CI)

Synonyms: o-Terphenyl (8CI); 1,1'-Biphenyl, 2-phenyl-; 1,2-

Diphenylbenzene

d. meta-Terphenyl

CAS No. 92-06-8

CA Index Name: 1,1':3',1"-Terphenyl (9CI)

Synonyms: m-Terphenyl (8CI); 1,1'-Biphenyl, 3-phenyl-; 1,3-

Diphenylbenzene; 1,3-Terphenyl; 3-Phenyl-1,1'-biphenyl; m-

Diphenylbenzene; m-Triphenyl;

e. para-Terphenyl

CAS No. 92-94-4

CA Index Name: 1,1':4',1"-Terphenyl (9CI)

Synonyms: p-Terphenyl (8CI); 1,1'-Biphenyl, 4-phenyl-; 1,4-

Diphenylbenzene; 4-Phenylbiphenyl; p-Diphenylbenzene; p-

Triphenyl;

## B. Manufacturing & Use

Members of the Polyphenyl (3- & 4-Phenyl Rings) Category, Mixed Terphenyls and Quaterphenyls are products originating from the same chemical manufacturing process. A polyphenyl stream consisting primarily of four or less aromatic rings is manufactured at a single US manufacturing site in an essentially closed, continuous process. This polyphenyl stream is processed through varying degrees of physical separation into commercial products which are either sold directly or used as site limited intermediates for further chemical reaction to manufacture other products. Nowhere in the process are 100 % mixed terphenyls or 100 % quaterphenyls isolated. All products manufactured and used as test articles for the studies described in this Test Plan, are combinations of terphenyls and quaterphenyls. Solutia does not isolate nor sell any of the individual terphenyl isomers (ortho-, meta- or para-) or any of the individual Quaterphenyl isomers in other than small volume, research or product development quantities.

Solutia Inc. historically has marketed three products from this singular process. One product, sold under the tradenames SANTOWAX R ® and THERMINOL 88 ® contains a high (81:17) Mixed Terphenyl:Quaterphenyl ratio. A second product, sold as THERMINOL 75® (also known as MCS-1980 during earlier product development) possesses a lower (62:34) Terphenyls:Quaterphenyl ratio, although Mixed Terphenyls are still the predominant chemical species. Both Mixed Terphenyl products are predominantly mixtures of meta- and para-terphenyl isomers, with only very small amounts (< 10%) of the ortho- isomer present. A third product, sold as SANTOTAR 9 ® or SANTOWAX Q ® consists primarily (90% Quaterphenyls: 10% Terphenyls) of Quaterphenyls.

A TLV ® of 5.0 mg/m³ (ceiling) has been established for Terphenyls (ACGIH, 2002) in order to protect against possible ocular, dermal, and respiratory tract irritation; human responses to terphenyls have been characterized as "relatively low" with no adverse effects detected in a work force except irritation (Beard and Noe, 1982). Only a few employees are involved in the manufacturing operation and have minimal potential for skin or airborne exposure, which occurs chiefly during material transfer operations. Specific manufacturing procedures and practices have been established to minimize occupational exposure potential, especially as these materials are handled under high temperature conditions which could cause thermal burns.

While individual terphenyl isomers have reportedly been used as solvents or even consumer products, no such uses are known to pertain to the mixed isomer products currently sold by Solutia. Essentially all of Solutia's current commercial products containing Mixed Terphenyls and Quaterphenyls are used as heat storage and transfer agents in closed systems in the industrial setting. Loss to the atmosphere or from non-POTW aqueous streams during manufacturing or processing is minimal and only by

accident. Hence, very limited occupational or environmental exposure is expected to occur.

## II. CATEGORY JUSTIFICATION

For purposes of the HPV Challenge Program, EPA has provided guidance as to the definition and justifications to be used in selection of a chemical Category (US EPA, 1999c). The definition states that a chemical Category should be "a group of chemicals whose physicochemical and toxicological properties are likely to be similar or follow a regular pattern as a result of structural similarity". Solutia Inc. has opted to form the Polyphenyl (3- & 4-Phenyl Rings) Category with this guidance in mind.

#### Common Structure

Each of the two chemical substances selected for inclusion in this category is a mixture of aromatic hydrocarbons containing 3 and 4 benzene rings, respectively. The products formed during manufacturing are separate streams originating from the same manufacturing process. Each product which served as a test article in the data presented in this Test Plan is one of mixed chemicals containing varying amounts of differing isomeric forms of the two base chemicals: terphenyls (polyphenyls with 3 open phenyl rings) and quaterphenyls (polyphenyls with 4 open phenyl rings). The difference between the Mixed Terphenyls streams and the Quaterphenyls stream lies in the amount of isomeric forms of the terphenyl components versus the amount and isomeric forms of quaterphenyls found within each substance. Mixed Terphenyls contain higher levels of 3-ring moieties (generally in the 60-90% range) and lesser 4ring structures (10-30%) while other Quaterphenyls contain high levels (80-90%) of 4-ring structures and lower (10-20%) levels of 3-ring moieties. Throughout this Test Plan the terms "Mixed Terphenyls" and "Quaterphenyls" will refer to these commercial mixtures rather than to the chemicals as described by the specific CAS numbers (unless otherwise noted). Hence, both entities within this Category are of common structure.

## Common Functional Groups

Each of these Polyphenyls are aromatic hydrocarbons containing a mixture of either 3 or 4 noncondensed benzene rings without any additional functional constituents added. The position (either *ortho* to, *meta* to, or *para* to each other) of the ring placement of the secondary or tertiary benzene rings is the only structural difference between the various isomers.

### Similar or even Identical Properties or Hazards

While there are substantive differences in the physicochemical properties of the individual terphenyl and quaterphenyl isomers, the mixed isomeric forms are less distinctive. Their physical form ranges from crumbly, partially waxy-like to completely waxy at room temperature. Increased molecular weights of the 4-phenyl ring quaterphenyls renders greater waxiness, lower volatility and higher boiling

points. Other parameters are similar, but not identical. A summary of available physicochemical data can be found in Table 3.

Environmental Fate data are summarized in Table 4. Whether measured or estimated, there appears close agreement in each of the HPV Endpoints recorded for members of this Category, as they all possess qualities reflective of their condensed ring structures.

Comparative aquatic toxicity of the members of this Category can be found in Table 5. As shown, a similar degree of toxicity has been observed across the multiple test species included in this dataset.

Table 6 summarizes the comparative mammalian toxicity of these chemicals. Comparative review indicates a similar degree of toxicity between both Category members for all endpoints.

Thus, similarities in the degree of toxicity and the extensive comparative data sets presented for the Mixed Terphenyls and the Quaterphenyls support use of a Category approach for these chemicals.

### III. TEST PLAN RATIONALE

The information obtained and included to support this Test Plan has come from either 1) internal studies conducted by/or for Solutia Inc. (or its predecessor Monsanto Co.), 2) has been extracted from the scientific literature either as primary references or as found in well-accepted, peer-reviewed reference books, or 3) were estimated using environmental models accepted by the US EPA (1999b) for such purposes. This initial assessment includes information on physicochemical properties, environmental fate, and human and environmental effects associated with each of the two Mixed Terphenyls products sold by Solutia as well as the commercial Quaterphenyls product of this Category. The data used to support this program include those Endpoints identified by the US EPA (1998); key studies have been identified for each Endpoint and summarized in Robust Summary form and included in Section VII of this dossier. Thus, we have consolidated test results from both Mixed Terphenyl products into one Robust Summary and have generated a second Robust Summary to include data on Quaterphenyls. As these substances are, themselves, mixtures of isomeric forms, we have chosen to develop separate Robust Summary data packages for each of the three Terphenyl isomers (ortho, meta, and para) as Surrogates. Information available on these Surrogates has been used as Supplemental to support existing data needs through "read across" or further corroborate data developed on Mixed Terphenyls.

All Environmental, Ecotoxicity and Mammalian Toxicity studies were reviewed and assessed for reliability according to standards specified by Klimisch *et al* (1997), as recommended by the US EPA (1999a). The following criteria were used for codification:

- Reliable without Restriction Includes studies which comply with US EPA and/or OECD-accepted testing guidelines, which were conducted using Good Laboratory Practices (GLPs) and for which test parameters are complete and well documented,
- 2. Reliable with Restriction Includes studies which were conducted according to national/international testing guidance and are well documented. May include studies conducted prior to establishment of testing standards or GLPs but meet the test parameters and data documentation of subsequent guidance; also includes studies with test parameters which are well documented and scientifically valid but vary slightly from current testing guidance. Also included were physical-chemical property data obtained from reference handbooks as well as environmental endpoint values obtained from an accepted method of estimation (i.e. EPIWIN).
- 3. Not Reliable Includes studies in which there are interferences in either the study design or results that provide scientific uncertainty or where documentation is insufficient.
- 4. Not Assignable This designation is used in this dossier for studies which appear scientifically valid but for which insufficient information is available to adequately judge robustness.

Those studies receiving a Klimisch rating of 1 or 2 are considered adequate to support data assessment needs in this Dossier. Those key studies selected for inclusion are considered typical of the Endpoint responses observed in other studies of a similar nature and design, which were identified during our search of the literature.

## IV. TEST PLAN SUMMARIES AND CONCLUSIONS

The referenced available data for each Category member has been placed in an Endpoint-specific matrix and summarized individually in Table 1 (Mixed Terphenyls) and Table 2 (Quaterphenyls). Generally, data exists for each Category Member to evaluate its potential hazards in this screening level assessment. Where an HPV Endpoint has been identified as untested, the need for testing has been assessed (1) with the understanding that these chemicals behave in a similar and/or predictable manner, and (2) by interpolation (i.e. Read-Across technique) between data from other key studies already available either with the mixture or from a Surrogate. Thus, we have used preexisting data, where possible, to support our assessment of potential hazards of the chemicals in this Category and avoid the unnecessary testing of additional laboratory animals.

Conclusion: Nearly all HPV Endpoints have been satisfied for the Mixed Terphenyls and Quaterphenyls with data from studies that were either well

documented, used OECD guideline methods and conducted in accord with GLPs, or were estimated from acceptable estimation modeling programs. Use of the "Read Across" technique was employed to support a limited number of Quaterphenyl Endpoints. No HPV Endpoint data was identified for assessment of the Reproductive Toxicity for either Category member. Hence, a single Reproductive Toxicity Screen (OECD 421) is proposed with Mixed Terphenyls. The use of the "read across" technique to assess Quaterphenyls for this Endpoint is planned, to avoid the unnecessary testing of animals.

Physical-chemical property values - Physicochemical values for nearly all Endpoints were obtained for commercially available Mixed Terphenyls and Quaterphenyls. Thus, these values were given a classification of "2-Reliable with restrictions". Where no values were found, estimates have been made for Mixed Terphenyls and Quaterphenyls from accepted models. Use of these models to estimate other physico-chemical properties provided good concordance with known values for individual Mixed Terphenyls isomers. Thus, they have been given a classification of "2-Reliable with restrictions".

Environmental Fate values describing Transport (Fugacity) and Photodegradation for Mixed Terphenyls and Quaterphenyls were obtained using a computer estimation –modeling program (EPIWIN, 2002) recommended by EPA and classified as "2-Reliable with restrictions". Biodegradation data for each of the Category members were characterized in well documented studies and conducted in a design similar to OECD test #302 guidance. These studies thus are classified as "2-Reliable with restrictions". No Stability in Water (hydrolysis) data were found for either Mixed Terphenyls or Quaterphenyls. Based on their chemical structure, it can be reasonably expected that both Mixed Terphenyls and Quaterphenyls are resistant to hydrolysis; thus, additional testing is unwarranted.

**Ecotoxicity** – Acute Fish, Invertebrate and Plant (Algal) Toxicity Endpoints for Mixed Terphenyls have been fulfilled with studies that were conducted according to US EPA test guidance consistent with OECD test guidelines. All studies were well documented and were designated "2-Reliable with restrictions". An Acute Invertebrate Toxicity study, also designated as "2-Reliable with restrictions" has been included for Quaterphenyls. The Acute Fish and Algal Toxicity Endpoints for Quaterphenyls are fulfilled using the 'Read Across' method of data evaluation to that developed for Mixed Terphenyls, as no fully reliable studies were found in these two areas. Utility of this methodology is strengthened by comparative use of estimation modeling data for Mixed Terphenyls and individual Terphenyl isomers.

**Mammalian Toxicity** Endpoints, including Acute Toxicity, Repeated Dose Toxicity, Ames Mutagenicity and Chromosomal Aberration Testing for Mixed Terphenyls have been fulfilled by way of tests that either conformed directly to OECD test

guidance or followed test designs sufficient to assess toxicity. Thus, they have been designated either "1-Reliable without restriction" or "2-Reliable with restrictions".

An adequately conducted ("2-Reliable with restrictions") Acute Toxicity study has been conducted with Quaterphenyls from which a similar order of toxicity is observed as seen with Mixed Terphenyls. No Ames or Cytogenetics Mutagenicity studies or Repeated Dose Toxicity were identified for Quaterphenyls. However, based on structural similarity and composition of Mixed Terphenyls tested for these endpoints, these Endpoints for Quaterphenyls have been filled using the "Read Across" technique for data assessment.

No adequately conducted study has been identified to assess reproductive toxicity for either Mixed Terphenyls or Quaterphenyls. Thus, we propose to conduct an OECD 421 Reproductive/Developmental Toxicity screen for Mixed Terphenyls and utilize "Read Across" methods for Quaterphenyl evaluation, thus minimizing the number of animals to be tested.

Based on the conclusions as outlined above on HPV Endpoint assessment, following is a tabular depiction of data availability and testing recommendations for Mixed Terphenyls (Table 1) and Quaterphenyls (Table 2).

Table 1. Test Plan Matrix for Mixed Terphenyls

	Info. Avail.	OECD	GLP	Other Study	Estimat. Method	Accept- Able ?	Testing Recomm.
PHYSICAL							
CHEMICAL							
Melting Point	Y	N	N	Y	N	Y	N
Boiling Point	Y	N	N	Y	N	Y	N
Vapor Pressure	Y	N	N	Y	N	Y	N
Partition Coefficient	Y	N	N	Y	N	Y	N
Water Solubility	Y	N	N	Y	N	Y	N
ENVIRONMENTAL							
FATE ENDPOINTS							
Photodegradation	Y	N	N	N	Y	Y	N
Stability in Water	N	-	-	-	-	Y	N
Biodegradation	Y	N	N	Y	N	Y	N
Transport between	Y	N	N	N	Y	Y	N
Environmental							
Compartments							
(Fugacity)							
ECOTOXICITY							

Acute Toxicity to	Y	N	Y	Y	N	Y	N
Fish							
Acute Toxicity to	Y	N	Y	Y	N	Y	N
Aquatic Invertebrates							
Acute Toxicity to	Y	N	Y	Y	N	Y	N
Aquatic Plants							
MAMMALIAN							
TOXICITY							
Acute Toxicity	Y	Y	Y	Y	N	Y	N
Repeated Dose	Y	N	N	N	N	Y	N
Toxicity							
Genetic Toxicity –	Y	Y	Y	Y	N	Y	N
Mutation (Ames)							
Genetic Toxicity –	Y	Y	Y	Y	N	Y	N
Chromosomal							
Aberrations							
Reproductive	N	-	-	-	-	N	Y
Toxicity							

Y = Yes; N = No; C = Read-Across from Isomers (o-, m-, and p-); - = Not applicable

Table 2. Test Plan Matrix for Quarterphenyls

	Info. Avail.	OECD	GLP	Other Study	Estimat.  Method	Accept- Able ?	Testing Recomm.
PHYSICAL CHEMICAL							
Melting Point	Y	N	N	Y	N	Y	N
Boiling Point	Y	N	N	Y	N	Y	N
Vapor Pressure	Y	N	N	Y	N	Y	N
Partition Coefficient	Y	N	-	-	Y	Y	N
Water Solubility	Y	N	Y	Y	N	Y	N
ENVIRONMENTAL FATE ENDPOINTS							
Photodegradation	Y	-	-	-	Y	Y	N
Stability in Water	N	-	-	-	-	Y	N
Biodegradation	Y	N	N	Y	N	Y	N
Transport between Environmental Compartments (Fugacity)	Y	-	-	N	Y	Y	N
ECOTOXICITY							

Acute Toxicity to	N	-	-	С	Y	Y	N
Fish							
Acute Toxicity to	Y	Y	Y	N	Y	Y	N
Aquatic Invertebrates							
Acute Toxicity to	N	-	_	С	Y	Y	N
Aquatic Plants							
MAMMALIAN							
TOXICITY							
Acute Toxicity	Y	N	N	N	N	Y	N
Repeated Dose	N	-	-	С	-	Y	N
Toxicity							
Genetic Toxicity –	N	-	-	С	_	Y	N
Mutation (Ames)							
Genetic Toxicity –	N	-	_	С	-	Y	N
Chromosomal							
Aberrations							
Reproductive	N	-	_	-	-	N	С
Toxicity							

Y = Yes; N = No; R = Reputable Reference; ; - = Not applicable

C = Read-Across from available data or new testing on Mixed Terphenyls

## V. Data Set Summaries and Evaluations

The key studies used in this assessment to fulfill the HPV requirements for Mixed Terphenyls and Quaterphenyls have been placed in an Endpoint-specific matrix, and further discussed below. Additionally, we have provided reference to similar studies conducted with one or more component isomeric forms, which have been included in the discussions below. Robust Summaries for each study referenced, whether it be for the Mixed isomer component or the individual isomers, can be found in Section VII of this dossier.

## A. Chemical/Physical Properties

Measured values are available for most of the **Physical-Chemical** properties associated with Solutia's Mixed Terphenyls commercial products and can be found in Table 3. A calculated value, using an EPA recommended methodology, for each Endpoint has been included for comparative purposes and confirms good agreement between calculated and measured values. Thus, these values are considered "2-Reliable with restrictions". In most cases, measured values, obtained from either reputable references or from internal studies, have also been obtained for each of the 3 terphenyl isomers predominant in Mixed Terphenyls. Visual inspection of these values provides corroborating support for

values provided for Mixed Terphenyls. A Robust Summary has been prepared for each of the references included in Table 3.

Similar to the Mixed Terphenyls, measured physical-chemical properties have been located for Solutia's Quaterphenyls commercial product. Additionally, we have provided values for each physical-chemical Endpoint using estimation models recommended by EPA and that were used to derive values for Mixed Terphenyls and its isomers. Where measured data are not available, it is reasonable to assume that models providing accurate values for 3-phenyl ring compounds (terphenyls) would also provide similarly useful values for 4-phenyl ring compounds (the quaterphenyls). Hence, these estimations also are considered "2-Reliable with restrictions" and fulfill the data needs for Quaterphenyls.

In summary, Mixed Terphenyls and Quaterphenyls are solid, waxy-like entities at room temperature and possess exceedingly low vapor pressures. Waxiness, and hence Boiling and Melting Point, increase as vapor pressure decreases even further with the addition of another phenyl ring (between terphenyls and quaterphenyls) and as molecular weight increases. Mixed Terphenyls have a relatively high measured partition coefficient which is quite similar to its estimated value; as expected, Quaterphenyls have an even higher calculated value. All water solubility values, for Mixed Terphenyls, its isomeric components and the Quaterphenyls, establish this category of chemicals as possessing very low (< 0.1 ppm) water solubility.

Conclusion: Sufficient data exists to characterize the Physical-Chemical properties of the Mixed Terphenyls and Quaterphenyls. Measured values were corroborated by comparing estimated and measured values and then were compared to similar values obtained for each of the 3 isomeric forms of Terphenyls found in Mixed Terphenyls. Thus, all HPV data requirements for this Endpoint have been met and no further data collection is planned.

Table 3. Selected Physical Properties of Polyphenyls (3- & 4-Phenyl Rings) and Surrogates

Chemical	Boiling Pt. (°C.)	Melting Pt. (° C.)	Vapor Pressure (hPa @ 25 °C)	Water Solubility (mg/L)	Partition Coefficient (Log Kow)
Mixed Terphenyls CAS No. 26140-60-3	376 deg. C (calculated)	210.1 deg. C. (calculated)	0.00000412 (calculated)	0.215 mg/L (calculated)	5.52 (calculated)
SANTOWAX R ® Mixed Terphenyls (81% Terphenyls; 17% Quaterphenyls)	364	145		0.11	5.21 (calculated)
THERMINOL 75 ® Mixed Terphenyls (62% Terphenyls; 34 % Quaterphenyls)	343	76	0.0000081	0.151	6.03 5.16 (calculated)
o-Terphenyl (Surrogate) CAS No. 84-15-1	332	56.2	0.0003	1.24	5.28 (measured) 5.52 (calculated)
m-Terphenyl (Surrogate) CAS No. 92-06-8	363	87	0.0000233	1.51	5.52 (calculated)
p-Terphenyl (Surrogate) CAS No. 92-94-4	376	210.1	0.000000456 (calculated)	0.0018	6.03 (measured)  5.52 (calculated)
Quaterphenyls CAS No. 29036-02-0	481.2 (calculated)	184.1 (calculated)	0.0000000023 (calculated)	0.0068 (calculated)	7.28 (calculated)
SANTOTAR 9 ® Quaterphenyls (90% Quaterphenyls, 10% Terphenyls)	> 420	200		0.002	

Category members emboldened type; Surrogate chemicals in normal type.

## C. Environmental Fate and Biodegradation

Shake-flask Ultimate Biodegradability studies have been conducted to assess the biodegradation potential of Mixed Terphenyls and Quaterphenyls; they have been summarized in the Robust Summary section of this Dossier and cited in Table 4 below. While each study was conducted prior to inception of standardized international guidelines for **Biodegradability** testing and GLPs, they followed similar standards for conduct subsequently codified into OECD guideline 302 and GLP documentation. Thus,

they are each considered "2-Reliable with restrictions". A Semi-Continuous Activated Sludge (SCAS) assay with Mixed Terphenyls is also included as it was well documented and thus also considered "2-Reliable with restrictions". For comparative purposes, similar Shake Flask studies and a River Die Away study with the three terphenyl isomers are provided as supplemental information and summarized in Section VII. Studies confirm that Mixed Terphenyls and Quaterphenyls undergo very slow biodegradation.

A single, comparative study of the photochemical reactions associated with each of the three terphenyl isomers has been summarized in the Robust Summary section of this dossier. This study has been classified as "2-Reliable with restrictions", as it provides useful Supplemental information, appears well conducted, but did not conform to codified OECD guidelines. Comparative values have been included in Table 4. No photodegradation testing was found for Mixed Terphenyls. However, based on the limited photodegradation exhibited by each of these terphenyl isomers, little appreciable photodegradation of the Mixed Terphenyls is expected to occur. Based on a "Read Across" approach using these results from its predominant isomers, this HPV Endpoint for Mixed Terphenyls is considered adequate. AOPWIN modeling for this **Photodegradation** Endpoint has also been included for comparative purposes and has been coded as "2-Reliable with restrictions".

Estimation of **photolysis** of Quaterphenyls through use of a model similar to that employed for Mixed Terphenyls also indicates little, if any, likelihood of photolysis. This study is also considered "2-Reliable with restrictions". Based on model estimation and structural similarity to Mixed Terphenyls, there would appear to be no need to further establish this Endpoint experimentally.

We have incorporated the use of an estimation model (EPIWIN, 2002) for determination of Transport Between Environmental Compartments (**Fugacity**), for Mixed Terphenyls and Quaterphenyls, as well as the terphenyl surrogate isomers. A Fugacity Level III model was used in each case, and employed measured values, where possible, as recommended by the US EPA. Thus, the estimations derived from each of these models have been classified as "2-Reliable with restrictions". These estimates have also been included in Table 4 and are cited in the Robust Summary section of this Dossier; data entries used in the Level III fugacity model have been included in the Robust Summaries for validation of output.

No values have been identified to define the **Stability in Water** (hydrolysis) of any of these Polyphenyls. Further no such values could be calculated using EPIWIN (2002) as each chemical has only aromatic rings and no functional groups, and thus form structures which are listed in Lyman et al. (1990) as "Generally Resistant to Hydrolysis". Thus, "[t]esting for Stability in Water is not needed for substances generally recognized to have molecular structures or possess only functional groups that are generally known to be resistant to hydrolysis" (OECD, 2002).

Conclusion: Sufficient information exists to characterize the Environmental Fate and Biodegradation of each of these Polyphenyls. Where experimental data do not

exist, employing "Read Across" techniques or using an estimation model (AOPWIN and EPIWIN) recommended by EPA provided necessary information; in one case (hydrolysis) the rational lack of need for testing has already been recognized. Thus, all HPV data requirements for these Endpoints are met and no further data collection is planned.

To summarize, this Category of chemicals would not be expected to normally enter the aquatic environment, as the products which contain these chemicals are not intended to be discharged to the environment. However, their limited entry could be envisioned after incidental spills and equipment leakage. Thus, the Environmental fate of these Polyphenyls, based on Fugacity modeling of the members of this Category, is expected to be focused primarily in the soil and sediment as main environmental target compartments. None of these chemicals is readily hydrolysable, all have exceedingly low water solubility characteristics, and would be expected to undergo limited photolysis in the environment. As part of the soil or sediment, these chemicals are expected to extensively degrade. In soil studies with Mixed Terphenyls, extensive biological degradation occurred in soils studies with T Waves ranging between 8-12 weeks. Additionally, rapid primary biodegradation of the two most water-soluble Terphenyl isomers occurred in River Die Away tests, once acclimation ensued.

Table 4. Comparison of Environmental Fate Endpoints for Category Members

Chemical	Biodegradation Rate	Stability in Water	Photodegradation (% Disappeared- 29 days Irradiation)	Fugacity (%)
Mixed Terphenyls CAS No. 26140-60-3		Not susceptible to hydrolysis	Half-life = 27.9 hrs (calculated)	Air - 1.05% Water- 12.0% Soil- 43.8% Sediment- 43.1%
SANTOWAX R ® Mixed Terphenyls (81% Terphenyls; 17% Quaterphenyls)	11.5% Mean Disappearance in SCAS	Not susceptible to hydrolysis		
THERMINOL 75 ® Mixed Terphenyls (62% Terphenyls; 34 % Quaterphenyls)	7-10% Theoretical CO2 formed-Shake Flask Ultimate Biodegradation	Not susceptible to hydrolysis		
o-Terphenyl (Surrogate) CAS No. 84-15-1	20 % Theoretical CO2 formed- Shake Flask Ultimate Biodegradation	Not susceptible to hydrolysis	< 8 (measured) Half-life = 27.9 hrs (calculated)	Air- 1.29% Water- 14.7 % Soil- 50.9 % Sediment-33 %
m-Terphenyl (Surrogate) CAS No. 92-06-8	38 % Theoretical CO2 formed- Shake Flask Ultimate Biodegradation	Not susceptible to hydrolysis	14 (measured) Half-life = 20.3 hrs (calculated)	Air- 0.87% Water- 11.8 % Soil- 45 % Sediment- 42.4 %
p-Terphenyl (Surrogate) CAS No. 92-94-4	10 % Theoretical CO2 formed in Shake Flask Ultimate Biodegradation	Not susceptible to hydrolysis	< 10 (measured) Half-life = 27.9 hrs (calculated)	Air- 1.06% Water- 11.7 % Soil- 45.3 % Sediment-41.9 %
Quaterphenyls CAS No. 29036-02-0		Not susceptible to hydrolysis	Half-life = 13.8 hrs (calculated)	Air- 0.22% Water- 3.47 % Soil- 32.3 % Sediment-64 %
SANTOTAR 9 ® Quaterphenyls (90% Quaterphenyls, 10% Terphenyls)	7 % Theoretical CO2 formed in Shake Flask Ultimate Biodegradation	Not susceptible to hydrolysis		

Category members emboldened type; Surrogate chemicals in normal type.

## D. Aquatic Toxicity

Experimental data have been found with Mixed Terphenyls for all three aquatic toxicity Endpoints. In each case, a well conducted study, following international testing and GLP guidance has been summarized in Table 5 and further described in the Robust Summary section of this dossier. In each case, these studies are considered "2-Reliable with restrictions". Also reported in the Robust Summary section of this dossier are the results of an Early Lifestage chronic fish study with Mixed Terphenyls using Fathead Minnows, which has be classified as "1-Reliable without restriction". The NOEC of 0.037 mg/L reported in that study is also consistent with the degree of toxicity exhibited in acute studies with other aquatic species. Both measured and estimated values for acute aquatic toxicity of each of the three Mixed Terphenyls isomers are also reported in Table 5. These values are consistent with values obtained for the Mixed Terphenyls products. This Supplemental data has been summarized in the respective Robust Summary section of this dossier.

Experimental results for all three species compare favorably with estimated values using the ECOSAR model. In all cases, Mixed Terphenyls exhibit a high degree of aquatic toxicity.

An acute Daphnia study, considered "2-Reliable with restrictions" has been conducted with Quarterphenyls. It too is indicative of a high degree of toxicity, as seen with Mixed Terphenyls. No acute fish or algal studies have been located for Quaterphenyls. However, in as much as the Invertebrate study confirms its high aquatic toxicity potential, as does ECOSAR modeling (which gave good congruence between experimental and modeled estimates for these endpoints with Mixed Terphenyls) for acute fish and algal toxicity, it is concluded that no additional acute aquatic testing is needed to confirm the self evident, that Quaterphenyls possess a degree of aquatic toxicity similar to that observed with Mixed Terphenyls across aquatic species.

Conclusion: Sufficient data exists to characterize the Acute Aquatic Toxicity properties of each of these Polyphenyl Category members. All HPV data requirements for this Endpoint have been met with acceptable empirical data for Mixed Terphenyls. We have used accepted, validated estimation models coupled with experimental data for Quaterphenyl to provide information needed such that no further data collection is required for either of these materials.

Table 5. Comparison of Aquatic toxicity parameters for Category members and Surrogates

Chemical	Fish LC 50 (mg/L) (96-hr)	Chronic Fish NOEC (mg/L)	Invertebrate (Daphnia) EC50 (mg/L) (48-hr)	Algae EC50 (mg/L) (96-hr)
Mixed Terphenyls CAS No. 26140-60-3	0.028 (calculated)		0.039 (calculated)	0.031 (calculated)
SANTOWAX R ® Mixed Terphenyls (81% Terphenyls;	27 (R. trout)		0.27	0.015 (chlorophyl a) 0.020 (cell number)
17% Quaterphenyls)				
THERMINOL 75 ® Mixed Terphenyls (61% Terphenyls;	> 0.75 (P. promelus)	0.037	0.043	0.103 (cell number)
34% Quaterphenyls)				
o-Terphenyl (Surrogate) CAS No. 84-15-	0.084 (calculated)		0.045 (measured) 0.115 mg/L (calculated)	0.088 (calculated)
m-Terphenyl (Surrogate) CAS No. 92-06-	0.084 (calculated)		0.022 (measured) 0.115 mg/L (calculated)	0.088 (calculated)
p-Terphenyl (Surrogate) CAS No. 92-94-	0.028 (calculated)		> 5.5 (measured - exceeded water solubility) 0.039 mg/L (calculated)	0.031 (calculated)
Quaterphenyls CAS No. 29036-02-0	0.002 (calculated)		>0.069 (measured)  0.004 (calculated)	0.003 (calculated)

Category members emboldened type; Surrogate chemicals in normal type.

## D. Mammalian Toxicity

## 1.0 Acute Toxicity

Key acute toxicity studies by the oral exposure route for Mixed Terphenyls and Quaterphenyls are included in Table 6. Each study was conducted specifically or in general agreement with OECD acute toxicity testing guidance and are considered "1-Reliable without restriction" and "2-Reliable with restrictions", respectively. The Mixed Terphenyl study cited was conducted with a 99%:1% Terphenyl-to-Quaterphenyl mixture which was high in meta- and para- isomers, and low (<1%) in ortho-terphenyl. Additional acute rat oral toxicity studies, conducted with a lower ratio of terphenyls-to-quaterphenyls (61% terphenyls:34% quaterphenyls) have been included in Table 6 and cited in the Robust Summary section of this dossier.

Acute rat oral LD50 values for each of the three terphenyl isomers found in Mixed Terphenyls were found in the literature (Cornish, Bahor and Ryan, 1962), are reported in Table 6, and are summarized as Supplemental information in the Robust Summary section of this dossier.

Conclusion: Sufficient data from well-documented studies (Acute Oral Toxicity) exist to meet the Acute Toxicity data set requirements for Mixed Terphenyls and Quaterphenyls. Hence, no further acute toxicity testing is planned.

Table 6. Acute Mammalian Toxicity for Category members

Chemical	Rat Oral LD50 (mg/kg)	Repeated Dose (Oral studies)	Mutagenicity Salmonella Test	Cytogenetics
SANTOWAX MP ® Mixed Terphenyls CAS No. 26140-60-3 (>99 % Terphenyls)	> 5,000			
SANTOWAX OM ® Mixed Terphenyls CAS No. 26140-60-3 (96 % Terphenyls; 4 % Quaterphenyls)	1400	235-d rat chronic: NOEL= 3 mg/kg/d		
SANTOWAX R ® Mixed Terphenyls (81% Terphenyls; 17% Quaterphenyls)			Negative without S-9 TA 1535, 1537, 1538, 98, 100 and D4 yeast; neg. with S9 in TA 1535, 1537, 1538, 98; pos. TA 100  Negative: +/- S-9 CHO/HGPRT Assay	Negative -CHO cell cytogenicity assay +/- S-9
THERMINOL 75 ® Mixed Terphenyls (61% Terphenyls; 34 % Quaterphenyls)	2604		Negative +/- S-9 TA 1535, 1537, 1538, 98, 100 and D4 yeast Negative: +/- S-9 CHO/HGPRT Assay	Negative: rat bone marrow in vivo assay
o-Terphenyl (Surrogate) CAS No. 84-15-1	1,900	30-d rat: NOEL=100 mg/kg	Neg-strain TM667 +/- S-9	
m-Terphenyl (Surrogate) CAS No. 92-06-8	2,400	30-d rat: NOEL=100 mg/kg	Neg-strain TM667 +/- S-9	
p-Terphenyl (Surrogate) CAS No. 92-94-4	> 10,000	30-d rat: NOEL=250 mg/kg		
SANTOWAX Q ® Quaterphenyls CAS No. 29036-02-0 (95 % Quaterphenyls; 5 % Terphenyls	5,650			

Category members emboldened type; Surrogate chemicals in normal type.

## 2.0 Repeated Dose Toxicity

A chronic rat study with Mixed Terphenyls has been published in the scientific literature and is cited in Table 6. While conducted well before development of OECD test guidelines or GLPs, this study is considered sufficient to meet this HPV Endpoint, for it greatly exceeds the minimum duration necessary for consideration and has included most of the testing endpoints included in those guidelines. Based on the thoroughness of its design and duration, this study is considered sufficient to evaluate the repeated dose toxicity of Mixed Terphenyls and thus has been judged as "2-Reliable with restrictions".

This study used a test material consisting of 95% Terphenyls and 5% Quaterphenyls. By comparison, this material was higher in the ortho-terphenyl isomer content (64% ortho-) than found in commercial Mixed Terphenyls, which contain <2% ortho-isomer. Based on 30-day oral rat studies conducted with each of the Terphenyl isomers (Table 6), the ortho-isomer is considered quantitatively similar in toxicity to the meta-terphenyl isomer; comparatively, the para-isomer appears relatively of lesser toxicity. Effects on body weight and organ weights were observed after 30-days of treatment with either the o- or m- isomer and each produced a NOEL of 100 mg/kg day (Table 6). As each of the commercial Mixed Terphenyls contains significant amounts of meta-isomer (> 55%), their repeated dose toxicity can be expected to be similar to that of the material used in this chronic study.

No repeated dose toxicity studies have been found for Quaterphenyls. However, based on the similarity of structure and physical properties between the Mixed Terphenyls and Quaterphenyls, a similarity of biological response would be anticipated. Thus, rather than conduct of unnecessary additional repeated dose toxicity testing, use of the "Read across" technique has been employed to render the need for similar testing with Quaterphenyls unnecessary.

### **Conclusion:**

Based on conduct of an acceptable chronic oral rat study with Mixed Terphenyls and assessment of 30-day oral rat studies with each of the three Terphenyl isomers, the Repe ated Dose Toxicity HPV Endpoint for Mixed Terphenyls is complete. While no studies were found for Quaterphenyls, use of "Read across" for Quaterphenyls negates the need for additional testing for this Endpoint.

## 3.0 Mutagenicity and Chromosomal Aberrations

## Ames Test

Three Ames point mutation studies have been conducted with Mixed Terphenyls. Two studies were conducted with THERMINOL 75 (61% Terphenyl:36% Quaterphenyl) and one with SANTOWAX R (81% Terphenyl:17% Quaterphenyl). All studies conformed to

OECD Test Guideline 471, athough only one (with THERMINOL 75) was conducted in accord with GLPs. Thus, the two studies conducted prior to inception of GLPS are considered "2-Reliable with restrictions" while the other is considered "1-Reliable without restriction". All three studies have been summarized in the Robust Summary of this dossier. Two studies reported no mutagenic response in any of the 5 Salmonella tester strains used, with or without metabolic activation. The third study reported a positive response only in TA100 with, but not without, metabolic activation. No mutagenic responses were observed in other Salmonella strains used. Weight-of-evidence among these three studies would indicate that Mixed Terphenyls do not elicit a genotoxic response in this assay. Further confirmation of a lack of Genotoxicity via point mutations can be found in the results of two mammalian cell point mutation studies with THERMINOL 75 and SANTOWAX R. No mutagenic activity was observed in either of two independently conducted CHO/HGPRT mammalian forward mutation assays (Solutia, 1984a, Solutia, 1986a). Robust Summaries of each of these studies has been included in this dossier.

No point mutation assays have been found evaluating Quaterphenyls. Using the "Read Across" methodology, we believe it appropriate to apply results reported above which was obtained from testing Mixed Terphenyl fractions containing substantive amounts of Quaterphenyls.

Conclusion: The Ames Test Category Endpoint for each of the Category members has been met and no further testing should be considered for the gene point mutation Endpoint.

#### Chromosomal Aberrations -

An *in vitro* CHO cell chromosomal aberration study has been conducted with an 81:17 ratio of Terphenyls:Quaterphenyls (SANTOWAX R) following a study design similar to OECD Test guideline 473. The study was well documented and followed GLPs and thus is considered to be "1-Reliable without restriction". Additionally, an *in vivo* mouse bone marrow cytogenetics assay has been conducted with a 62:34 ratio of Terphenyls:Quaterphenyls (THERMINOL 75). It, too, conforms to OECD testing guidance (guideline no. 475) and is considered "1-Reliable without restriction". These studies have been used to fulfill this HPV Endpoint for Mixed Terphenyl. Each study has been referenced in Table 6 and summarized in the Robust Summary section of this dossier. No evidence of chromosomal aberrations were observed in either study.

No chromosomal aberration studies have been located with Quaterphenyl. Using the "Read Across" methodology, we believe it appropriate to apply results reported above obtained for Quaterphenyls.

Conclusion: On the basis of reliable *in vitro* and *in vivo* Chromosomal Aberration Assays available for Mixed Terphenyls and use of "Read Across" for Quaterphenyls in lieu of unnecessary testing, this HPV Endpoint has been fulfilled.

### 5. Reproductive and Developmental Toxicity

No reliable evaluation of reproductive parameters has been found either in the open literature or in search of in-house files for either Mixed Terphenyls or Quaterphenyls.

Reproductive organs were evaluated in a chronic rat study reported for Mixed Terphenyls in the Repeated Dose section of this dossier. No effects were noted either in organ weights or weight ratios or following histopathological evaluation of testes or ovaries following 235 days of oral exposure up to 350 (male)/409 (female) mg/kg/day Mixed Terphenyls. Similarly, no effects on rat gonads were reported following 30 days of oral exposure to m-, p-, or o-terphenyl. Thus, there is no evidence that Mixed Terphenyls or Quaterphenyls would be expected to affect reproductive performance.

A single mouse *in vitro* fertilization study with each of the 3 Terphenyl isomers was found in the literature. Due to deficiencies in design this study has been classified for reliability as "3- Not reliable". However, it has been included in the Robust Summary section of each Terphenyl isomer as Supplemental information.

Conclusion: In light of the ambiguity of the *in vitro* experimental data addressing the potential of individual Terphenyl isomers to affect reproductive outcome, we are prepared to conduct a Reproductive/developmental toxicity screen test (OECD 421) with Mixed Terphenyls. With results obtained from this study, the "Read Across" technique will be applied to Quaterphenyls, in order to minimize the unnecessary use of additional animals.

### VI. REFERENCES

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## VII. ROBUST STUDY SUMMARIES

Study Summaries Appended for Mixed Terphenyls and Quaterphenyls, and also o-, m-, and p-Terphenyl.

## IUCLID

## **Data Set**

 Existing Chemical
 : ID: 26140-60-3

 CAS No.
 : 26140-60-3

 EINECS Name
 : terphenyl

 EC No.
 : 247-477-3

 TSCA Name
 : Terphenyl, Mixed

Molecular Formula : C18H14

Producer related part

Company : Solutia Inc.
Creation date : 17.03.2003

Substance related part

Company : Solutia Inc. Creation date : 17.03.2003

Status : Memo :

Printing date : 23.07.2003

Revision date

Date of last update : 23.07.2003

Number of pages : 34

**Chapter (profile)** : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 **Reliability (profile)** : Reliability: without reliability, 1, 2, 3, 4

Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),

Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1. General Information

ld 26140-60-3 **Date** 23.07.2003

1.0.1	APPLICANT AND COMPANY INFORMATION
1.0.2	LOCATION OF PRODUCTION CITE IMPORTED OR FORMUL ATOR
1.0.2	LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR
1.0.3	IDENTITY OF RECIPIENTS
1.0.4	DETAILS ON CATEGORY/TEMPLATE
1.1.0	SUBSTANCE IDENTIFICATION
1.1.1	GENERAL SUBSTANCE INFORMATION
1.1.2	SPECTRA
1.2	SYNONYMS AND TRADENAMES
1.3	IMPURITIES
1.4	ADDITIVES
1.5	TOTAL QUANTITY
1.6.1	LABELLING
1.6.2	CLASSIFICATION
1.6.3	PACKAGING
1.7	USE PATTERN
1.7.1	DETAILED USE PATTERN
4 7 2	MET IODO OF MANUFACT IDE
1.7.2	METHODS OF MANUFACTURE

## 1. General Information

ld 26140-60-3 **Date** 23.07.2003

1.8	REGULATORY MEASURES
1.8.1	OCCUPATIONAL EXPOSURE LIMIT VALUES
1.8.2	ACCEPTABLE RESIDUES LEVELS
1.8.3	WATER POLLUTION
1.8.4	MAJOR ACCIDENT HAZARDS
1.0.4	WIAJOR ACCIDENT HAZARDS
1.8.5	AIR POLLUTION
1.8.6	LISTINGS E.G. CHEMICAL INVENTORIES
1.9.1	DEGRADATION/TRANSFORMATION PRODUCTS
1.9.2	COMPONENTS
1.10	SOURCE OF EXPOSURE
1.11	ADDITIONAL REMARKS
1.11	
1.12	LAST LITERATURE SEARCH
1.13	REVIEWS

ld 26140-60-3 **Date** 23.07.2003

### 2.1 MELTING POINT

**Value** : 76 - °C

Sublimation

Method : other: Internal assay

Year : 1983
GLP : no
Test substance : other TS

Remark : Beginning of slurry point with range of 76-80 deg. C.
Test substance : THERMINOL 75 consisting of 62 % Mixed Terphenyls, 34 %

Quaterphenyls and 4 % High Boilers

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

09.07.2003

**Value** : 145 - °C

Sublimation

Method : other: Monsanto internal assay

Year : 1980 GLP : no Test substance : other TS

Remark : Pour point

**Test substance** : Santowax R consisting of 81% Mixed Terphenyls, 17% Quaterphenyls and

2% High Boilers.

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

09.07.2003 (2)

**Value** : =  $210.1 - {^{\circ}C}$ 

Sublimation :

Method : other: calculated (MPBPWIN v1.40)

Year : 2003 GLP : no Test substance : other TS

**Test substance**: Terphenyl [CAS No. 26140-60-3]

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

09.07.2003 (3)

#### 2.2 BOILING POINT

**Value** : 343 - °C at

Decomposition

Method : other: Internal assay

Year : 1983
GLP : no
Test substance : other TS

**Test substance** : THERMINOL 75 consisting of 62 % Mixed Terphenyls, 34 %

Quaterphenyls and 4 % High Boilers

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

09.07.2003 (1)

ld 26140-60-3 **Date** 23.07.2003

**Value** : 364 - °C at

Decomposition

**Method** : other: Internal assay

Year : 1980 GLP : no Test substance : other TS

Test substance : SANTOWAX R consisting of 82 % Mixed Terphenyls, 16 % Quaterphenyls

and 2 % High Boilers.

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

09.07.2003

Value :  $= 376 - ^{\circ}C$  at

Decomposition

Method : other: calculated (MPBPWIN v1.40)

Year : 2003 GLP : no Test substance : other TS

**Test substance**: Terphenyl [CAS No. 26140-60-3]

**Reliability** : (2) valid with restrictions

09.07.2003 (3)

#### 2.3 DENSITY

#### 2.3.1 GRANULOMETRY

#### 2.4 VAPOUR PRESSURE

**Value** : .0000081 - hPa at 25 °C

Decomposition

**Method** : other (measured)

Year : 1982 GLP : no data Test substance : other TS

Method : Internal technical analysis

**Test substance**: THERMINOL 75 consisting of 62 % Mixed Terphenyls, 34 %

Quaterphenyls and 4 % High Boilers

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

09.07.2003 (5)

**Value** : = .00000412 - hPa at 25 °C

Decomposition :

**Method** : other (calculated)

Year : 1985
GLP : no
Test substance : other TS

Remark : Reported as 3.09 x 10e-6 mm Hg @ 25 deg. C

**Test substance**: Terphenyl [CAS No. 26140-60-3]

**Reliability** : (2) valid with restrictions

09.07.2003 (6)

ld 26140-60-3 **Date** 23.07.2003

#### 2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water Log pow : = 6.03 - at °C

pH value :

Method : other (measured): not reported

Year : 1993
GLP : no data
Test substance : other TS

**Test substance**: Therminol 75 consisting of 62% Mixed (2% ortho-, 55% meta-, 5 % para-)

Terphenyls, 34 % Quaterphenyls and 4 % High Boilers.

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

09.07.2003

Partition coefficient : octanol-water Log pow : 5.16 - at °C

pH value :

Method : other (calculated)

**Year** : 1990

GLP :

**Test substance** : other TS

**Method** : Calculated method using equation Log Kow = 5.00-0.67 (log water

solubility), based on Chiou et al 1977.

**Test substance**: THERMINOL 75 consisting of 62 % Mixed Terphenyls, 34 %

Quaterphenyls and 4 % High Boilers

**Reliability** : (2) valid with restrictions

09.07.2003 (8)

Partition coefficient : octanol-water Log pow : 5.21 - at °C

pH value :

**Method** : other (calculated)

**Year** : 1990

GLP

**Test substance**: other TS

**Method** : Calculated method using equation Log Kow = 5.00-0.67 (log water

solubility), based on Chiou et al 1977.

Test substance : Santowax R consisting of 81% Mixed Terphenyls, 17% Quaterphenyls and

2% High Boilers.

**Reliability** : (2) valid with restrictions

09.07.2003 (8)

**Partition coefficient** : octanol-water Log pow : = 5.52 -at  $^{\circ}C$ 

pH value : -

Method : other (calculated): atom/fragment contribution method

Year : 1995 GLP : no Test substance : other TS

Method : Individual atom/fragment contribution (AFC) values were determined for

130 simple chemical substructures. Another 235 correction factors were determined for various substructure orientations. The partition coefficient (log P) of a compound is estimated by summing all AFC values and

correction factors for a given chemical structure.

**Test substance**: Terphenyl [CAS No. 26140-60-3]

**Reliability** : (2) valid with restrictions

6/34

ld 26140-60-3 **Date** 23.07.2003

09.07.2003 (9)

### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water

**Value** : = -.151 mg/l at 25 °C

pH value : -

concentration : at °C

Temperature effects

Examine different pol.

**pKa** : at 25 °C

Description : Stable : Deg. product :

Method : other
Year : 1982

GLP : no data
Test substance : other TS

Method : Measured, saturated column method. Test material was coated at the 5%

level on 89/100 mesh Chromosorb WHP, which was then loaded into the saturator column. The concentration of test substance in the solution (test water was deionized MilliQ water) leaving the saturator column was measured using a coupled column LC technique fitted with a UV detector. Four separate runs were made varying flow through rate (1 or 2.3 mL/min)

and total volume collected (either 5 or 10 mL).

**Result** : 0.151 +/- 0.013 mg/L at 25 deg. C.

**Test substance** : Test substance was MCS-1980 consisting of 61% Mixed Terphenyls, 34%

Quaterphenyls, and approx. 4% High Boilers.

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

23.06.2003 (10)

Solubility in : Water

**Value** : - .11 mg/l at 23 °C

pH value : -

concentration : at °C

Temperature effects :

Examine different pol. :

**pKa** : at 25 °C

Description : Stable : Deg. product : Method :

Year : 1979
GLP : no
Test substance : other TS

**Method**: Presumed similar to methods used for MCS 1980.

Test substance : SANTOWAX R consisting of 82 % Mixed Terphenyls, 16 % Quarterphenyls

and 2 % High Boilers.

**Reliability** : (2) valid with restrictions

09.07.2003 (11)

Solubility in : Water

**Value** : = .215 - at 25  $^{\circ}$ C

pH value : -

concentration : at °C

Temperature effects : Examine different pol. :

ld 26140-60-3 **Date** 23.07.2003

**pKa** : at 25 °C

**Description** : slightly soluble (0.1-100 mg/L)

Stable

Deg. product

Method : other: calculated

Year : 1996
GLP : no
Test substance : other TS

Method : Estimation performed using regression equations based on log Kow

values.

Test substance : Terphenyl [CAS No. 26140-60-3].

**Reliability** : (2) valid with restrictions

09.07.2003 (12)

### 2.6.2 SURFACE TENSION

### 2.7 FLASH POINT

### 2.8 AUTO FLAMMABILITY

### 2.9 FLAMMABILITY

### 2.10 EXPLOSIVE PROPERTIES

### 2.11 OXIDIZING PROPERTIES

### 2.12 DISSOCIATION CONSTANT

### 2.13 VISCOSITY

### 2.14 ADDITIONAL REMARKS

ld 26140-60-3 **Date** 23.07.2003

### 3.1.1 PHOTODEGRADATION

Type : other

Light source

**Light spectrum** : - nm

Relative intensity : - based on intensity of sunlight

Deg. product :

Method : other (calculated): AOPWIN v1.90

Year : 2003 GLP : no Test substance : other TS

**Remark**: Vapor phase mixed terphenyls are susceptible to reaction with

photochemically produced hydroxyl (OH) radicals. The 2nd order rate constant for reaction with hydroxyl radicals was calculated as 9.1946E-12 cm3/(molecule\*sec). Based on 1.5E6 OH molecules/cm3 and assuming 12 hours of sunlight per day, the estimated photo-oxidation half-life is 27.9

hours

**Test substance**: Terphenyl [CAS No. 26140-60-3]

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

16.06.2003 (13)

### 3.1.2 STABILITY IN WATER

Remark : The test substance (Terphenyl) is not susceptible to hydrolysis. It has only

3-membered aromatic rings associated with its structure, which are listed in

Lyman in Table 7.1 - Types of Organic Functional Groups That Are

Generally Resistant to Hydrolysis. Lyman, WJ, Reehl, WF and Rosenblatt,

DH. 1990. Handbook of Chemical Property Estimation Methods. Environmental Behaviour of Organic Compounds. American Chemical

Society, Washington, DC.

02.06.2003

3.1.3 STABILITY IN SOIL

### 3.2.1 MONITORING DATA

### 3.2.2 FIELD STUDIES

### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III

Media : other: air-water-soil-sediment

Air : 1.05 % (Fugacity Model Level I)

Water : 12 % (Fugacity Model Level I)

Soil : 43.8 % (Fugacity Model Level I)

Biota : % (Fugacity Model Level II/III)

Soil : 43.1 % (Fugacity Model Level II/III)

Method : other

ld 26140-60-3 **Date** 23.07.2003

Year : 2003

**Method**: Used EPIWIN, Syracuse Research Corp. The following physical properties

of Mixed Terphenyls were used as the model input parameters: water solubility=0.215 mg/L, vapor pressure = 3.09E-6 mm Hg; log Kow = 5.52; melting point = 210 Deg C. All property values were taken from this

Robust Summary Dossier.

**Remark**: Air: half life = 27.9 hr; emissions = 1000 kg/hr

Water: half life = 900 hr; emissions = 1000 kg/hr Soil: half life = 900 hr; emissions - 1000 kg/hr Sediment: half life = 3600 hr; emissions - 0 kg/hr

Persistence Time: 993 hr

Test substance : Mixed Terphenyls
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

09.07.2003

### 3.3.2 DISTRIBUTION

### 3.4 MODE OF DEGRADATION IN ACTUAL USE

### 3.5 BIODEGRADATION

Type : aerobic

**Inoculum** : domestic sewage

Deg. product :

Method: otherYear: 1974GLP: noTest substance: other TS

Method : Semicontinuous activated sludge test. Twenty six (26) week test, 24-h

cycle of draw and fill, weekly analyses of parent material using UV absorbance, while metabolites were quantified using GC -FID, 1 mg (week 1), 3 mg (week 2) and 5 mg (thereafter) of TS was added per cycle, activated sludge mixed liquor from municipal sewage treatment plant was inocula, a series of 3 hexane off gas scrubbers were used to catch

olatiles

**Result** : Overall mean daily disappearance rate was 11.5 +/- 7.2%. GC analyses

showed that the several peaks that make up the TS degraded at varying levels. Analyses showed complete loss of o-terphenyl, a halving of m-terphenyl concentration, and little change in p-terphenyl concentration. No

volatile losses were reported.

Test substance : THERMINOL 88, a mixture of 81% Mixed Terphenyls, 17 % Quaterphenyls

and 2% Higher Boilers.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

02.06.2003 (14)

Type : aerobic

**Inoculum** : domestic sewage

Deg. product

Method : other: CO2 Shake Flask

Year : 1980 GLP : no Test substance : other TS

ld 26140-60-3 **Date** 23.07.2003

(15)

Method

: Used 50-day Shake Flask Ultimate Biodegradation study design. Two tests were performed, a 50-day test using an inoculum acclimated for 30 days. Test medium was a standard BOD medium enhanced with 2 times normal amount of phosphate buffer; 4 times normal amount of FeCL3, and 40 mg (NH4)2SO4 per liter purfied water. Two liter triplicate flasks were fitted with barium hydroxide solution to catch CO2; glucose positive control,and then inoculum from aclimated solution were prepared using a 16 or 30 days SCAS procedure: activated aerated, suspended solids of 3000 mg/L, 24-h at the end of which it was settled for 30 min, 1L decanted, 1 L raw sewage added containing test substance. Initial bacterial counts in inoculum during SCAS preparation averaged 4.0E+6 and 3.1+6 CFU/ml. in the first and second tests respectively. Initial test substance was a nominal 20 mg/L. Analyzed using HPLC for test material remaining. Test vessels were incubated at 27+/-deg. C.in the dark on a rotary shaker.

Result

The positive control averaged approximately 100% thCO2. For the test using a 16-d inoculum, thCO2 formation averaged 7+/-3%. Chemical analyses at experiment end showed that only 4 to 55% of the initial test substance remaining in the first test and < 1 percent in the second test. Thus, primary degradation is relatively rapid, while the biodegradation products are more persistent.

**Test substance** 

: MCS 1980, which contained a mixture of 63% Mixed Terphenyls, 35%

Quaterphenyls and 2% High Boilers.

**Reliability** 19.06.2003

(2) valid with restrictions

Type : aerobic

Inoculum

-

Contact time : 7.5 month

**Degradation** :  $94 - (\pm) \%$  after 7.5 month

Result

Deg. product

**Method** : other: soil bacterial degradation

Year : 1988
GLP : no
Test substance : other TS

Method

Used a defined methodology to determine the degree of biodegadability caused by soil microorganisms from two separate soil samples. Two concentrations of test material (50 ppm and 0.5 ppm) were prepared in methylene chloride. Two soil types, (1) Missouri Bottoms, a sandy soil with 0.5% organic carbon and a moisture content of 11.3% at 1/3 BAR and (2) Florida muck, a heavy loam containing 32.9% organic carbon and an 82% moisture content at 1/3 BAR. Soil samples containing test material were analyzed by HPLC after 0, 0.5, 1, 2, 4, 6, 8, 12, 15, and 32 weeks on study. A microtox screen was employed prior to study start to insure no bacterial toxicity would interfere with the subsequent test. Method of detection of test material was validated on both soils prestudy. Soil samples were stabilized prior to study start such that they contained a uniform level of microorganisms. Soil samples (25 gm) were placed in 125 ml jars and spiked with 250 ul of test solution containing the test material in solvent. Jars were capped and shaken, then lids removed and restirred manually. After being lightly recapped, the jars containing the test material and soil were incubated in the dark at 25 deg. C and 80% humidity until sampled. Three replicates of each treated group plus a control per time period per soil type were used. Sterile controls and matrix blanks were also employed. Kinetic parameters were calculated from raw data.

Remark : Provided as Supplementary information.

Result : % Reduction Relative to Nominal Concentration after 32 Weeks on Test

Nominal Conc. % Red. Soil Type % Vs Sterile Soil T 1/2 (weeeks)

500 ppm 94 Mq. Bott. 81 8.1

ld 26140-60-3 **Date** 23.07.2003

500 ppm 94 Mo. Bott. 81 8.1 0.5 ppm 75 Mo. Bott. - 16.0

500 ppm 84 Fla Muck 70 12.1 0.5 ppm 0 Fla Muck - no change

Terphenyl rapidly began to undergo biological degradation upon introduction to either sandy or loam soil types containing soil bacteria. Most of the loss observed was related to biological means although small differences in losses between untreated and sterile soil suggests some

abiotic causes are also involved.

**Test substance** : Test substance labeled "Terphenyl" containing a mixture of terphenyl

isomers.

**Reliability** : (2) valid with restrictions

09.07.2003 (16)

### 3.6 BOD5, COD OR BOD5/COD RATIO

### 3.7 BIOACCUMULATION

### 3.8 ADDITIONAL REMARKS

### 4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : static

**Species**: Pimephales promelas (Fish, fresh water)

**Exposure period** 96 hour(s) Unit mg/l > - .75 **NOEC** LC50 >= - .75 Method other : Year 1984 **GLP** yes Test substance other TS

Method : Design based on USEPA (1975) 660/3-75-009 Committee on Methods for

Toxicity Tests with Aquatic Organisms. Fathead minnows were obtained from inhouse cultures, held in tanks for 2 weeks under 16h light, 8h dark and fed commercial fish food until 48h before testing. Fish had a mean weight and length of 0.95 g and 45 mm, respectively. Static bioassay was performed in 20 L glass aquaria containing 15L of deionized reconstituted well water. Water quality of test dilution water at test initiation was: DO= 94-95% of saturation, pH=6.8-7.2, total hardness =28-34 mg/L CaCO3, total alkalinity of 26-28 mg/L CaCO3. Test water was maintained at 22 +/- 1 deg. C. in a water bath. Fish were held without food for 48 hr before testing and were not fed during the test. Nominal concentrations of 0.38,

0.75, 1.5 and 7.5 mg/L were prepared by adding test material to dimethylformamide. Test concentrations were not measured during the test. Test solutions were cloudy in all but the lowest concentration, signaling aqueous concentrations above the limit of solubility. Across all test vessels, DO ranged up to 8.6 mg/L, pH ranged between 6.7-7.5, and

temperature ranged from 22-23 deg. C.

**Result** : Deaths of 0-20% were reported for all test levels at 96-h. The aqueous limit

of sol ubility was estimated to be 0.75 mg/L. Since deaths ranged from 0 to 10% at the apparent limit of solubility the 96h LC50 value was considered

to be  $\Rightarrow$  0.75 mg/L. and the NOEC was  $\Rightarrow$  0.75 mg/L.

**Test substance**: Therminol 75 which consisted of 62% Mixed Terphenyls, and 34%

Quaterphenyls and 4% High Boilers.

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

02.06.2003 (17)

Type : static

**Species**: Salmo gairdneri (Fish, estuary, fresh water)

**Exposure period** : 96 hour(s) **Unit** : mg/l

LC50 : 27 - measured/nominal

Limit test : no
Analytical monitoring : no
Method : other
Year : 1979
GLP : yes
Test substance : other TS

Method : Used USEPA (1975) 660/3 -75-009 Committee on Methods for Toxicity Test

with Aquatic Organisms. Rainbow trout were obtained from a fish hatchery, held in culture tanks for 2 weeks under 16 h light, 8 hr dark. Fish were fed commercial fish food until 48 h before the test. Fish had a mean weight and length of 36 and 38.4 mm respectively, Static bioassays were performed in 5 gal glass vessels containing 15 L of laboratory well water, with 10 fish per concentration. Water quality of test dilution water at test

initiation: DO 8.9 mg/L, pH 7.8, total hardness 240 mg/l CaCO3 total alkalinity 360 mg/L CaCO3. Test water was maintained at 12 +/- 1 degree C in a water bath. Fish were held without food for 48 h before testing and were not fed during the test. Based on the results of a rangefinding test, test levels used were 5, 10, 21, 42, and 75 mg/L TS. Test material (vellow crystals) were mixed as a suspension in aetone, except in the two highest concentrations, which had Test Substance directly added to the water. Aliquots of the acetone suspension were added to the vessels to obtain the lower three nominal test concentrations. Water and TS were vigorously stirred. The compound was reported to precipitate and float in clumps in all test solutions, which is not surprising as the water solubility of this material is reportedly 0.15 mg/L. Actual test concentrations were not measured during the test. Across all test vessels DO ranged from 4.8-7.7 mg/L; pH ranged from 7.5 to 8.06; temperature remained at 12 degree C and ammonia remainded below the toxic limit. LC50 and CI were calculated using the methods of Litchfield and Wilcoxon (J. Pharm. Exp. Ther 96: 99-

113)

**Remark**: An initial test was also summarized in this study but has not been

considered in this assessment as spurious, non dose-related deaths were observed in all test concentrations assayed. Thus, a second, repeat study has been summarized above. Provided as Suppplemental information.

Result : 96-h LC50 = 27 mg/L (95% CI=20-37 mg/L). No control mortalities were

reported. At 24-h no mortality was observed while at 48-h no mortalities were reported in the lower 3 concentrations with partial mortalities up to 50% in remaining concentrations. At 96-h, there were mortalities ranging from 0 - 100% in a dose related manner across all test concentrations.

**Test substance** : THERMINOL 88, consisting of 82% Mixed Terphenyls, 16% Quaterphenyls

and 2% High Boilers.

Conclusion : No deaths were observed at levels of water saturation (low dose of 5 mg/L)

which exceeded the water solubility. This HPV endpoint is considered complete, using a previous acute fish study in conjuction with the Chronic

Fish robust summary cited in section 4.5.1.

**Reliability** : (2) valid with restrictions

19.06.2003 (18)

Туре

 Species
 : other: fish

 Exposure period
 : 96 hour(s)

 Unit
 : mg/l

 LC50
 : = .028

**Method** : other: calculated (EcoSAR)

Year

GLP : no
Test substance : other TS

Remark : An acute fish 96-h LC50 was calculated using ECOSAR, from the USEPA.

The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within

ECOSAR.Information supplied as Supplemental.

**Test substance**: Terphenyl [CAS No. 26140-60-3]

02.06.2003 (19)

### 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static

Species : Daphnia magna (Crustacea)

 Exposure period
 : 48 hour(s)

 Unit
 : mg/l

 NOEC
 : < -.006</td>

 EC50
 : = -.043

 Method
 : other

 Year
 : 1983

 GLP
 : yes

 Test substance
 : other TS

Method: Used EPA method 660/3-75-009. 1975. Ten 24-h old D. magna Straus

were tested at room temperature in a series of three replicates per test concentration. Test concentrations were 0.006, 0.012, 0.025, 0.05, 0.1 mg/mL, plus clean water and solvent (0.5 mL DMF) controls. Tests were conducted in well water from St Peters, MO. Test concentrations were not measured. Daphnids were not fed. Test vessels were not aerated. Tests were conducted in 250-mL beakers or jars containing 200 mL of solution. Dissolved oxygen was monitored to ensure the concentration did not fall below 2 mg/L before the end of the test. Water quality was measured according to SOPs for dissolved oxygen, pH, alkalinity, hardness and temperature and no significant changes were observed in any parameter. During the 48-h test, pH ranged from 7.65 to 7.9, DO ranged from 7.8 to 8.1 mg/L. Temperature averaged 21deg. C., alkalinity ranged from 295-306 mgL, and hardness ranged from 245 to 250 mg/L. The heavy metals and organochlorines that are routinely measured in the well water were presented in the appendices. At 48-h, there were 7% mortalities in the clean water and solvent controls. There were partial mortalilties in a dose response fashion across all test concentrations. The estimated EC50 and

95% CI were determined using EPA statistical procedures.

**Result** : 24-h EC50=>0.1 mg/L; 48-h EC50 (95%CL)=0.043 (0.029-0.074) mg/L.;

NOEC<0.006 mg/L. % immobilized per dose level used (mg/L) after treatment (24-h:48-h)= control (0%:7%), solvent control (0:7), 0.006 (20:33), 0.012 (0:20), 0.025 (7:37), 0.05 (10:53), and 0.1 (13:70).

**Test substance** : MCS 1980 consisting of 62% Mixed Terphenyls, 34% Quaterphenyls and

4% High Boilers.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

19.06.2003 (20)

Type : static

Species : Daphnia magna (Crustacea)

**Exposure period** 48 hour(s) Unit mg/l **NOEC** .056 -EC50 .27 -**Limit Test** : nο **Analytical monitoring** nο Method other Year 1979 : GI P : yes Test substance other TS

Method : Used EPA method (1975) 660/3-75-009Committee on Methods for Toxicity

Tests with Aquatic Organisms. Ten <24-h old D. magna Straus were selected from an in-house colony and tested at 20 +/-1 deg. C in a series of two replicates per test concentration. Test concentrations were 0.056, 0.10, 0.18, 0.32, and 0.56 mg/L, plus clean water and solvent (acetone) controls. Tests were conducted using well water from Columbia, Mo. Concentrations were not measured. Daphnids were not fed. Tests were conducted in 25-mL glass beakers containing 200 mL of solution. Dissolved oxygen was monitored to ensure the concentration did not fall below 2 mg/L before the end of the test. Water quality was measured for dissolved oxygen, pH, ammonia, and temperature. No significant change were observed in any parameter measured. LC50 and CI were calculated

using EPA statistical procedures.

Remark : Supplemental information as a previously cited study was used to fulfill

HPV requirement.

**Result** : The 24-h EC50 (95% CL) was 0.72 (0.58-0/89) mg/L; the 48-h EC50 (95%

CL) was 0.27 (0.21-0.35) mg/L. The NOEC was determined to be 0.056 mg/L. At 24-h, there were no deaths in controls or the lower 4 test concentrations. Clumping of daphnids was observed at the highest three concentrations. At 48-h, there were no deaths in controls or the lowest test concentration, partial deaths in the middle three test levels and 100% deaths in the highest concentration tested. Clumping of daphnids was observed in the highest three concentrations tested. The pH at test initiation was 7.9 and at 48 hrs was 8.3; the DO at 48 hrs was 9.1 mg/L and

at test initiation alkalinity and hardness were 368 and 255 mg/l,

respectively.

Test substance : THERMINOL 88 consisting of 82% Mixed Terphenyls, 16% Quaterphenyls

and 2% High Boilers.

**Reliability** : (2) valid with restrictions

19.06.2003 (21)

Type

Species : Daphnia sp. (Crustacea)

 Exposure period
 : 48 hour(s)

 Unit
 : mg/l

 LC50
 : = .039 

**Method** : other: calculated (EcoSAR)

Year :

GLP : no Test substance : other TS

Remark : An acute Daphnia 48-h LC50 was calculated using ECOSAR, from the

USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within ECOSAR. Data supplied as Supplemental information.

**Test substance**: Terphenyl [CAS No. 26140-60-3]

02.06.2003 (19)

### 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)

**Endpoint** : other **Exposure period** 96 hour(s) μg/l Unit **EC50** 15 -20 -EC50 (cell no.) Limit test nο : **Analytical monitoring** nο Method other Year 1979 **GLP** ves **Test substance** other TS

Method : Used USEPA (1971) Algal Assay Procedure: Bottle Test. National

Eutrophication Research Program, Pacific Northwest Water Laboratory, Corvallis, OR. Cultures were incubated at 24 +/- degree C under 4000 lux illumination during a 24-hr photoperiod. Triplicate culture flasks were employed for each of the test concentrations and controls used. Nominal test concentrations were 3.2, 5.6, 10, 32, and 56 micrograms/L. Both clean water and solvent controls were included. Dimethylformamide (DMF) was used as a cosolvent (0.05 mL/test flask). Test material was dissolved in DMF and directly added to the test vessels. Chlorophyl a was measured using a Turner Model 111 fluorometer. Cell counts were made using a hemacytometer and a Zeiss Standard 14 compound microscope. Specifics of the culture medium were not found. Results were analyzed using probit

analysis and regression analysis. Growth data were analyzed by Student's

t-test. PH was maintained between 7.2-7.5 during the test.

Result : Chlorophyl a: 24-h and 48-h EC50 were > 56 microgram/L; 72-h EC50= 29

(95% CI of 3.1-263) microgram/L; 96-h EC50 (95%CI)= 15 (2.8-76) microgram/L. Cell No. 96-h EC50 (95% CL)= 20 (4.7-86) microgram/L.

**Test substance** : Therminol 88 consisting of 81% Mixed Terphenyls, 17% Quaterphenyls

and 2% High Boilers.

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

19.06.2003 (22)

Species : Selenastrum capricornutum (Algae)

**Endpoint** other **Exposure period** 96 hour(s) Unit μg/l EC50 = 103 -Method other Year 1984 GLP no data Test substance other TS

Method : Endpoint evaluated was chlorophyll a, cell number. Cultures were

incubated at 22 +/- 1 deg. C. under 4600 lux illumination during a 24-h photoperiod. Triplicate culture flasks were employed for each of the test concentrations and controls used. Nominal test concentrations were 62.5, 125, 250, 500 and 1000 ug/L. Both clean water and solvent controls were included. Acetone was used as a cosolvent (0.05 mL per test flask). Test material was dissolved in acetone and directly added to the test vessels. Test material was not measured during the test. Cell counts were made using a hemacytometer and a Zeiss Standard 14 compound microscope. Beginning cell counts in the test flasks were 2.0E+4 cells/mL. Specifics of the culture medium were not provided other than stating that test medium was regular algal assay procedure medium. Results were analyzed using USEPA methods (moving average angle method). pH was maintained

between 7.0-7.6 during the test.

**Remark**: Information provided as Supplemental.

**Result** : Cell Number = 96-h EC50 of 103 (95% CI of 86-168) micrograms/L. **Test substance** : Therminol 75 consisting of 62% Mixed Terphenyls, 34% Quaterphenyls

and 4% High Boilers.

19.06.2003 (23)

**Species** : other algae: green algae

Endpoint :

 Exposure period
 : 96 hour(s)

 Unit
 : mg/l

 LC50
 : = .031 

Method : other: calculated (EcoSAR)

Year

GLP : no Test substance : other TS

Remark : An acute green algal 96-h LC50 was calculated using ECOSAR, from the

USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES

notations within ECOSAR.

Information provided as supplemental data in light of available acute

aquatic studies cited in this reference.

**Test substance**: Terphenyl [CAS No. 26140-60-3]

19.06.2003 (19)

### 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

### 4.5.1 CHRONIC TOXICITY TO FISH

**Species**: Pimephales promelas (Fish, fresh water)

**Endpoint** other Exposure period 34 day(s) Unit mg/l **NOEC** = .037 -**Analytical monitoring** yes Method other : Year 1986 GLP : yes Test substance : other TS

Method : Designed to study the early life stage toxicity in Fathead Minnows. < 1-

day old, fertilized embryos were taken from the in-house culture. Flow-through testing was conducted using a modified Brungs proportional diluter over the course of 34 days (including 30 days post hatch). Test solutions were replaced at a rate of 5 times daily. The water supply was local well water which had a range of hardness and alkalinity of 25-36 mg/L and 25-30 mg/L, respectively, as CaCO3. The pH range was 7.0-7.4 and the

specific conductance was 100-120 micromhos/cm.

Fifty embryos were placed into incubation cups, one of which was suspended in each duplicate test 20-L glass aquarium (filled with 15 L) per test concentration and controls. Cups were glass jars with 16-mesh Nitex screen bottoms. Incubation cups were gently oscillated using a rocker arm apparatus. Hatching was deemed complete when no more than 5 unhatched viable embryos remained in any incubation cup (day 4 of exposure). Percent hatch success and survival were recorded.

Forty live larvae were placed back into their aquaria (from the cups) for 30 days of exposure to assay survival and growth (length and weight). Illumination (16 hr light) was provided by Cool White and Grow Lux fluores cent lights (20-100 foot candles at water surface). Test water was maintained at 25 +/- 1 deg. C. Water quality (temperature, DO, pH, hardness) was measured periodically during the test.

Five concentrations (mean measured of 0.034, 0.037, 0.064, 0.12, 0.29 mg/L) and an acetone solvent control were used. Test concentrations were measured during the test using GC-FID. Larvae were fed live brine shrimp three times daily and twice daily on weekends. Aquaria were cleaned several times per week. Across all test vessels and throughout the test, DO varied between 7.6 to 8.2 mg/L, temperature was steady at 26 deg. C, hardness varied between 28 and 30 mg/L CaCo3, and pH varied between

6.3-7.5.

**Remark**: This study, in conjuction with previously reported acute a quatic studies,

provides sufficient information to fulfill the requirements of the HPV

program for this endpoint.

**Result** : No effects on hatching mortality or success as compared to controls were

observed in any test concentration. No effects on larval weight were observed at any test concentration. Survival of larvae and larvae lengths were reduced at 0.064 mg/L, but not at 0.037 mg/L. The overall NOEC for

this study was 0.037 mg/L.

Test substance : Therminol 75 consisted of 62% Terphenyls, 34% Quaterphenyls and 4%

High Boilers.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

# 19.06.2003 (24) 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS 4.6.2 TOXICITY TO TERRESTRIAL PLANTS 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS 4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES 4.7 BIOLOGICAL EFFECTS MONITORING

**Id** 26140-60-3

4. Ecotoxicity

4.8

**BIOTRANSFORMATION AND KINETICS** 

4.9 ADDITIONAL REMARKS

### 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

### 5.1.1 ACUTE ORAL TOXICITY

Type : other

**Value** : > 5000 - mg/kg bw

Species : rat

Strain : Sprague-Dawley
Sex : male/female

Number of animals : 10
Vehicle : other
Doses : 5000 mg/kg

Method : OECD Guide-line 401 "Acute Oral Toxicity"

Year : 1989 GLP : yes Test substance : other TS

Method : Limit test conducted using 5M and 5F SD rats 9-12 week old. Test material

was suspended in corn oil and dosed at a constant volume of 10 ml/kg by gavage on test day 1. Clinical signs of toxicty were recorded daily, body weights and food consumption were recorded on test day 0, 7 and 14 and all animals necropsied. Temperature, humidity and light cycle were

controled; food and water were given ad libitum.

Result : Preliminary range-find study using 1M and 1F rat per group, resulted in no

deaths at dosages of 1,000, 2,000 and 2,600 mg/kg. No deaths occurred in the Limit Test of 5,000 mg/kg. Some reductions in food consumption were noted during the first 4 days after dosing. One female lost weight after 7 days of testing, all other rats at this time point and all rats (including the 1F) gained weight after 14 days. A single animal exhibited urine staining, hypoactivity and unthrifty hair coat during the study. No abnormal

observations were noted at necropsy for any animal.

**Test substance**: Santowax MP consisting of: 99% mixed terphenyls (75% meta, 24 % para,

<0.5% ortho-isomer) and 1% quaterphenyls.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

29.04.2003 (25)

Type : LD50

**Value** : = 2604 - mg/kg bw

Species : rat

Strain : Sprague-Dawley
Sex : male/female

Number of animals : 50 Vehicle : other

**Doses** : 1,984, 2,500, 3,150, 3,969 and 5,000 mg/kg **Method** : OECD Guide-line 401 "Acute Oral Toxicity"

Year : 1981
GLP : yes
Test substance : other TS

Method : Groups of 5M and 5F young, adult SD rats were administered one of 5

single doses by gavage of test material in corn oil. Clinical signs of toxicity were recorded each day of the 14-day observation period. All animals were necropsied. Body weights were recorded on study day 0, 7 and 14. Food and water were given ad libitum while temperature, humidity and light cycle were controled. LD50 determination and 95% CI were calculated by

the Probit method of Finny, 1971.

**Result** : LD50 = 2,604 (95% CI 2247-2940) mg/kg. Occurrance of deaths (in

parentheses) at each dose level were: 1,984 mg/kg (1/10), 2,500 mg/kg (6/10),3,150 mg/kg (6/10), 3,969 mg/kg (10/10), and 5,000 mg/kg (10/10). Deaths occurred within 1-3 days. Sedation, ptosis and ataxia were observed only during the initial day of dosing. Diarrhea, lacrimation, and prostration were seen at later time points. At necropsy, signs were evident

of gastrointestinal distress, hemorrhaging and discoloration.

Test substance : MCS 1980 consisting of 62% Mixed (2% ortho-, 55% meta-, 5% para-

)Terphenyls, 34% Quaterphenyls and 4% High Boilers.

**Reliability** : (1) valid without restriction

02.06.2003

Type : LD50

**Value** : = 1400 - mg/kg bw

Species : rat

Strain : Sprague-Dawley
Sex : male/female

Number of animals

Vehicle

Doses : Method :

Method: otherYear: 1962GLP: noTest substance: other TS

**Method**: Groups of 5 rats were administered test material mixed in corn oil by

gavage in logarithmically increasing doses between 500-10,000 mg/kg. All survivors were necropsied at study term. LD50 calculated by method of

Weil.

**Remark**: Provided as supplemental information; results describe the acute oral

toxicity of the Mixed Terphenyl material containing a high o-isomer ratio and which was tested in a subsequent Chronic rodent study and reported

in section on Repeated Dose.

**Result** : LD50 = 1,400 mg/kg

**Test substance**: Santowax OM, consisting of 95% Mixed (64% ortho-, 23% meta-, and 6%

para-isomers) Terphenyls and < 5% Biphenyl.

**Reliability** : (2) valid with restrictions

13.05.2003

### 5.1.2 ACUTE INHALATION TOXICITY

### 5.1.3 ACUTE DERMAL TOXICITY

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

### 5.2.1 SKIN IRRITATION

### 5.2.2 EYE IRRITATION

### 5.3 SENSITIZATION

### 5.4 REPEATED DOSE TOXICITY

Type : Chronic Species : rat

Sex : male/female
Strain : Long-Evans
Route of admin. : oral feed
Exposure period : 235 days
Frequency of treatm. : daily
Post exposure period : yes

**Doses** : 0.01%, 0.1% and 1.0 %; equivalent to (males/females): 3/3.5 mg/kg/d;

31/37 mg/kg/d; and 350/409 mg/kg/d

Control group : yes, concurrent vehicle NOAEL : = 3.5 - mg/kg bw

 Method
 : other

 Year
 : 1965

 GLP
 : no

 Test substance
 : other TS

Method

Groups of 9 male and 9 female rats were administered feed containing either 0.01%, 0.1% or 1.0% test material for up to 235 days. Test material was suspended in corn oil before admix with powdered rat chow. A concurrent vehicle control group was employed. Food and water were provided ad libitum. Animals were housed in wire-mesh caging, 3 rats/cage. Body weights were recorded on day 0 and monthly thereafter; food consumption was also recorded. One third (3 M/3 F) of the rats from each dose group were sacrificed on study days 130, 188 and 235. In an attempt to ascertain reversibility of renal lesions, 3M and 3F fed 1.0% treated diet for 188 days were switched to untreated feed between study days 188 and 235. At final sacrifice, each animal had blood drawn for hematological examination and had its liver, kidneys and lungs weighed, along with a gross necropsy. Histopathologic examination of the following tissues was performed: brain, lungs, heart, stomach, intestines, liver, spleen, pancreas, kidneys, adrenals, urinary bladder, testes, ovaries, and bone. Hematology parameters measured were hemoglobin, hematocrit and white blood cell count. Statistical analysis of mean values for body weight, organ weight and hematology parameters was performed using a t-test. A paired-feeding study, comparing a separate group of 6 rats fed 1.0% treated diet with a feed restricted group of similar size was also performed.

Result

Mean food test article consumption values for the low, mid and high test group, by sex (M:F) were: 3 and 3.5 mg/kg/d, 31 and 37 mg/kg/d and 350 and 409 mg/kg/d. One female rat fed 1.0% diet died between test days 130-188. No treatment-related effects were observed at 0.01% (3/3.5 mg/kg/d) which is considered the NOEL for this study. At 0.1% (31/37 mg/kg/d) a small reduction in body weight was noted after study day 180 in both males and females. An unidentified pigment was observed in the cytoplasm of some renal tubular cells at this test level. At 1.0% (350/409 mg/kg/d) dramatically lower body weights were observed in both sexes through the first 188 days of testing. Once removed from treated feed, substantive recovery of weight and increased food consumption was observed; final body weights for this group still did not achieve control levels by the end of the study. A statistically significant increase in hemoglobin values was noted at the end of the study for both male and female rats given 1.0% test material in the diet. Rats of both sexes exhibited increased liver weights at the two earlier time points. At the 1.0% test level, rats of both sexes exhibited pathological changes of the kidney consisting of tubular obstruction and an irreversible interstitial nephritis with scarring at both the 130- and 188-day time points. Some signs of partial reversibility of renal lesions was observed in the postdosing study portion. During the paired-feeding study, weight gain was reduced such that this reduction appears test-article related rather than entirely accountable to

feed palatability.

**Test substance**: SANTOWAX OM, consisting of 95% Mixed Terphenyls (64% ortho-, 25%

meta- and 6% para-) and 5% biphenyl.

**Reliability** : (2) valid with restrictions

Despite some limitations, these scientifically valid studies assessing prolonged exposure to mixed terphenyls provide sufficient information to

complete this HPV endpoint.

Flag : Critical study for SIDS endpoint

13.05.2003 (26)

### 5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test

System of testing : Salmonella typhimurium strains TA98, TA100, TA1535, and TA1537

**Test concentration** : 0.01, 0.04, 0.2, 1.0, 2.0, 3.0, and 10 mg/plate

**Cycotoxic concentr.** : equal to or greater than 1 mg/plate

**Metabolic activation** : with and without

Result : positive
Method : other
Year : 1982
GLP : yes
Test substance : other TS

Method : Method used was plate incorporation assay based on Ames test methods

consistent with OECD 471. All tests were run in duplicate and three plates were assayed at each dosage for each run both with and without metabolic activation. The S-9 liver homogenates were prepared from male SD rats and CD-1 mice given Arochlor 1254. All tester strains were obtained from Dr. B. Ames. Sterile DMSO was used as the solvent and a solvent control was employed of 20 uL/plate DMSO. Positive controls used were: 2-aminoanthracene, 9-aminoacridine, benzo(a)pyrene, NaNo2 and 2-nitrofluorene. A positive response was determined upon observation of a statistically significant dose-response increase in revertant colonies. Bartlett's test was used for pairwise comparison to controls and dose response determined using regression analysis for log-log straight lines;

P<0.01 was used.

Result : Positive response with TA100 only with S9; no mutagenic increase with

other Salmonella strains with S9 or any strains (including TA100) without

S9.

**Test substance** : MCS 1980 consisting of 62% Mixed Terphenyls and 34% Quaterphenyls

and 4% High Boilers.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

02.06.2003 (27)

**Type** : Cytogenetic assay

System of testing : Chinese Hamster Ovary Cell In Vitro Assay

**Test concentration**: 37.5, 75 and 150 ug/ml

Cycotoxic concentr. : 150 ug/ml with S9 and 18.8 ug/ml without S9

**Metabolic activation**: with and without

 Result
 : negative

 Method
 : other

 Year
 : 1987

 GLP
 : yes

 Test substance
 : other TS

**Method** : Study conducted according to OECD study design, testing involved 2

separate tests with and without S9 fraction added. Fischer male rat Arochlor 1254-induced liver homogenate was used. Cell cultures were handled to prevent photolysis of Brdu-substituted DNA. Each test

23/34

consisted of concurrent solvent and positive controls and at least 3 dose levels. Cells were incubated in McCoy's 5A medium with test agent ranging between 8-26 hrs, colcemid added to arrest cell division and then harvested/processed. 50 first-division metaphase cells for each dose level in each replication were scored blind from prepared slides for each dose level. Classes of aberrations were recorded and included simple, complex and other abnormalities. Statistical analysis (Chi square pair-wise comparison test) was conducted on individual dose points; significance was determined as P<0.05. A positive response required a statistically significant increase in cells with aberrations or aberrations per cell. Positive controls used (cyclophosphamide and MMS) functioned as expected.

**Remark** : Provided as supplemental information since this chemical has also been

tested in an In Vivo Cytogenetics Assay (see subsequent chapter 5.6)

Result : No increase in chromosomal aberrations was observed at any dose level at

any time point. A top dose level of 150 ug/ml was used as this proved to be the limit of solubility of test material in the solvent (acetone) of choice.

**Test substance** : Santowax R consisting of 81% Mixed Terphenyls and 17% Quarterphenyls

and 2% High Boilers.

**Reliability** : (1) valid without restriction

02.06.2003 (28)

**Type** : Bacterial reverse mutation assay

System of testing : Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538, and

Saccharomyces yeast D4

**Test concentration** : 0.1, 1.0, 10, 100 and 500 ug/plate

Cycotoxic concentr. : 500 ug/plate produced evidence of chemically-induced effect; low dose

was without demonstratable toxic effect.

**Metabolic activation**: with and without

 Result
 : negative

 Method
 : other

 Year
 : 1977

 GLP
 : no

 Test substance
 : other TS

Method : Study consistent with OECD 471, using plate overlay method. Duplicate

runs conducted, but not run in triplicate. Positive controls used were: MNNG, NF, QM, Anthrace, AAF, and AMQ. Test material dissolved in DMSO. Used S9 fraction obtained from liver of male rats given Arochlor 1254. A response was considered positive in any tester strain, with or without metabolic activation, if 3 concentrations were at least 3X (2X for

TA98 and D4) concurrent control values.

Result : No mutagenic response observed in any Salmonella tester strains or the

D4 Yeast, with or without metabolic activation.

**Test substance**: CP 75052; laboratory synthesized sample of commercial product Therminol

75, consisting of 62% terphenyl, 34% quaterphenyl and 4% High Boilers.

**Reliability** : (2) valid with restrictions

02.06.2003 (29)

**Type** : Bacterial reverse mutation assay

System of testing : Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538, and

Saccharomyces yeast D4

**Test concentration** : 0.1, 1.0, 10.0, 100, 500 ug/plate

**Cycotoxic concentr.** : 500 ug/plate produced evidence of chemically-induced effect; low dose

was without demonstratable toxic effect.

**Metabolic activation**: with and without

Result : negative

Method : other

Year : 1977

GLP : no

Test substance : other TS

Method : Study consistent with OECD 471, using plate overlay method. Duplicate

runs conducted, but got gun in triplicate. Positive controls used were:

runs conducted, but not run in triplicate. Positive controls used were: MNNG, NF, QM, Anthrace, AAF, and AMQ. Test material dissolved in DMSO. Used S9 fraction obtained from liver of male rats given Arochlor 1254. A response was considered positive in any tester strain, with or without metabolic activation, if 3 concentrations were at least 3X (2X for

TA98 and D4) concurrent control values.

Result : No mutagenic response seen in any Salmonella tester strain or D4 yeast,

with our without metabolic activation.

Test substance : CP 2321 SR (Santowax R) consisting of 81% Mixed Terphenyls and 17%

Quaterphenyls and 2% High Boilers.

**Reliability** : (2) valid with restrictions

02.06.2003 (30)

Type : HGPRT assay

System of testing : Chinese Hamster Ovary Cell line Test concentration : 5, 25, 50, 75, and 100 ug/ml

Cycotoxic concentr. : 100 ug/ml

Metabolic activation : with and without

Result : negative

Method : OECD Guide-line 476

Year : 1984
GLP : yes
Test substance : other TS

Method : CHO cell cultures, prepared from stock cultures originating from Dr. AW

Hsie, Oak Ridge National Laboratories, were introduced to flasks containing a density of approximately 5X10E5 cells/flask. After incubation in medium for 16-24 hr cells were removed, washed and 5 ml serum free medium F12, transferred into flasks and test material added directly, diluted in acetone. 1 ml S-9 fractions of male SD rat liver (Arochlor 1254-induced) homogenates (0, 1, 2, 5, and 10%) were added as appropriate. Flasks were gassed with CO2 and incubated for 5 hrs., then medium aspirated, washed and then reincubated an additional 19 hr. Colonies were subcultured in 0.05% trysin solution, cell no. counted and 1000 cells/ml subcultured; 0.2 ml aliquots were plated for survival. Cultures were incubated for up to 7 days and clones fixed, stained and counted for mutant selection. A preliminary cytotoxicity study was run using a range of 7 doses between 0.33 ug/ml-1000 ug/ml and 4 levels of S-9. A Preliminary study using dosages of 20, 50 and 100 ug/ml with and without S9 (0, 1, 2, 5, and 10%) was conducted in duplicate. A Confirmatory test was conducted using final concentrations of 5, 25, 50, 75 and 100 ug/ml with and without 10% S9. Positive controls used were: Ethylmethane sulfonate and Dimethyl nitrosamine. Untreated and solvent-treated controls were also run concurrently. This test was run in triplicate. Statistical treatment of raw data was performed using a computer program obtained from J.Irr (EPA) to evaluate mutation frequency. One way ANOVA was used on transformed mutation frequency data according to methodology supplied by Snee and

Irr (1981). p<0.01.

Remark : Supplementary information regarding the lack of genotoxicity observed in a

mammalian cell line point mutation as say.

Result : Cytotoxicity was complete at 333 ug/ml and significant at 100 ug/ml. No statistically significant differences in mutation frequency between treated

statistically significant differences in mutation frequency between treated and control doses were observed with or without any of the S9 fractions used. A dose-dependent treand was noted in cells treated with 10% S9 in the Preliminary Study. In the Confirmatory Study, no statistically significant increases in mutation frequency or trend were observed either with our without 10% S9. Positive and negative controls performed as expected.

Test substance : MCS 1980 consisting of 62% Mixed Terphenyls, 34% Quaterphenyls and

4% High Boilers.

**Reliability** : (2) valid with restrictions

23.07.2003 (31)

ld 26140-60-3 5. Toxicity Date 23.07.2003

Type **HGPRT** assay

System of testing Chinese Hamster Ovaries cells

Test concentration 10, 50, 100, 250, & 500 ug/ml (without S9); 1, 5, 10, 25, 50, 75, and 100

ug/ml (with S9)

Cycotoxic concentr. 16.7 ug/ml and higher Metabolic activation with and without

Result negative

Method OECD Guide-line 476

Year 1986 GLP : yes Test substance other TS

Method CHO cell cultures, prepared from stock cultures originating from Dr. AW

> Hsie, Oak Ridge National Laboratories, were introduced to flasks containing a density of approximately 5X10E5 cells/flask. After incubation in medium for 16-24 hr cells were removed, washed and 5 ml serum free medium F12, transferred into flasks and test material added directly, diluted in acetone. 1 ml S-9 fractions of male SD rat liver (Arochlor 1254-induced) homogenates (0, 1, 2, 5, and 10% S9) were added as appropriate. Flasks were gassed with CO2 and incubated for 5 hrs,, then medium aspirated, washed and then reincubated an additional 19 hr. Colonies were subcultured in 0.05% trysin solution, cell no. counted and 1000 cells/ml subcultured; 0.2 ml aliquots were plated for survival. Cultures were incubated for up to 7 days and clones fixed, stained and counted for mutant selection. A preliminary cytotoxicity study was run using a range of 8 doses between 0.167 ug/ml-500 ug/ml and 4 levels of S-9. A Preliminary study, using dosages of 5, 10 and 25 ug/ml with 1% & 2% S9 as well as 5, 50, 100 and 500 (without S9) ug/ml each with and without 5 and 10% S9, was conducted in duplicate. A Confirmatory test was conducted using final concentrations of 5, 25, 50, 75 and 100 ug/ml with 5% S9 and 1, 5, 10, 25. 50, 75, and 100 ug/ml in the absence of S9. Positive controls used were: Ethylmethane sulfonate and Dimethyl nitrosamine. Untreated and solventtreated controls were also run concurrently. This test was run in triplicate. Due to unfavorable response in the positive control, this experiment was conducted three times before minimum acceptable standards were met. Statistical treatment of raw data was performed using a computer program obtained from J.Irr (EPA) to evaluate mutation frequency. One way ANOVA was used on transformed mutation frequency data according to

methodology supplied by Snee and Irr (1981). p<0.01.

mammalian cell line point mutation assay.

Result Cytotoxicity was seen at 16.7 ug/ml and limits of solubility exceeded at test

levels of 167 and 500 ug/ml; deminished cytotoxicity appeared at doses fo 50 and 100 ug/ml in the presence of S9. No statistically significant differences in mutation frequency between treated and control doses were observed with or without any of the S9 fractions used. Similarly, in the Confirmatory Study, no statistically significant increases in mutation frequency or trend were observed either with our without 1-10% S9. Positive and negative controls performed as expected in the definitive

Supplementary information regarding the lack of genotoxicity observed in a

Confirmatory study.

**Test substance** Santowax R

Reliability (2) valid with restrictions

27.05.2003 (32)

### **GENETIC TOXICITY 'IN VIVO'**

Remark

Type Cytogenetic assay

**Species** rat

Sex male/female Strain Fischer 344

Route of admin. : i.p.

**Exposure period** : once with sampling periods of 6, 12 and 24 hrs. **Doses** : 500, 2500, and 5,000 mg/kg body weight

Result : negative

Method : OECD Guide-line 475 "Genetic Toxicology: In vivo Mammalian Bone

Marrow Cytogenetic Test - Chromosomal Analysis"

Year : 1985
GLP : yes
Test substance : other TS

Method : Dose levels selected based on pilot study were no effects were seen up to

5000 mg/kg test agent, the highest dose used in this study design. Six Fischer-344 rats/sex/time period were administered test agent in corn oil by intraperitoneal injection. Metaphase cells were collected from rat bone marrow (femur) at harvest times of 6, 12 and 24 hrs after treatment. Colchicine was administered 2 hr prior to sacrifice to arrest cells in c-metaphase. Marrow was exposed to hypotonic solution and fixed, cells and slides prepared and stained. All slides were coded before reading. Positive and negative (corn oil and untreated) controls were used for comparative purposes. Mitotic index was calculated based on counting of at least 1000 slides and chromosomal aberrations evaluated from at least 60 slides per animal per time point from the untreated control groups (male and female) and the 5,000 mg/kg test groups. All breaks, deletions, translocations and other changes were recorded. Mitotic Index, % chromosomally aberrant cells and frequency of chromosomal aberrations per cell were compared between treated vs control groups using ANOVA and Dunnett's test. P

< 0.05 was used.

Result : No toxicologically significant effects were noted at any dose level, nor

where there any deaths observed during the study. No increase in mitotic index, % aberrant cells or aberrations per cell were noted in either male or female rats evaluated after 6, 12, or 24 hrs following treatment at 5000

mg/kg test material.

**Test substance**: Therminol 7 5 consisting of 62% Mixed Terphenyls and 34% Quaterphenyls

and 4% High Boilers.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

02.06.2003 (33)

### 5.7 CARCINOGENICITY

### 5.8.1 TOXICITY TO FERTILITY

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

### 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Type : other In vitro/in vivo : In vivo Species : rat

Sex: male/femaleStrain: Long-EvansRoute of admin.: oral feedExposure period: 235 daysFrequency of treatm.: daily

Duration of test :

27/34

**Doses** : 0.01, 0.1 and 1.0 % (approx. 3/3.5, 31/37 and 350/409 mg/kg/d for males

and females, respectively)

**Control group** : yes, concurrent vehicle

Result : No histopathological effects noted on testes or ovaries after 130, 188 or

235 days of testing.

Method: otherYear: 1965GLP: noTest substance: other TS

**Remark**: This information has been summarized extensively in the Repeated Dose

Toxicity section of this monograph. While this data is insufficient for purposes of completely addressing this HPV endpoint, it does provide useful information indicative of a lack of histopathologic findings which

could affect reproductive performance.

**Test substance** : Santowax OM consisting of 95%Mixed Terphenyls (64% ortho-, 25% meta-

and 6% para-) and 5% biphenyl.

**Reliability** : (2) valid with restrictions

29.04.2003 (26)

### 5.9 SPECIFIC INVESTIGATIONS

### 5.10 EXPOSURE EXPERIENCE

### 5.11 ADDITIONAL REMARKS

# 6. Analyt. Meth. for Detection and Identification

ld 26140-60-3 **Date** 23.07.2003

- 6.1 ANALYTICAL METHODS
- 6.2 DETECTION AND IDENTIFICATION

# 7. Eff. Against Target Org. and Intended Uses

ld 26140-60-3 **Date** 23.07.2003

7.1	FUNCTION
7.2	EFFECTS ON ORGANISMS TO BE CONTROLLED
	ADALLIANA TA DE PROTESTED
7.3	ORGANISMS TO BE PROTECTED
7.4	USER
7.4	USER
7.5	RESISTANCE

# 8. Meas. Nec. to Prot. Man, Animals, Environment

ld 26140-60-3 **Date** 23.07.2003

8.1	METHODS HANDLING AND STORING
8.2	FIRE GUIDANCE
8.3	EMERGENCY MEASURES
8.4	POSSIB. OF RENDERING SUBST. HARMLESS
8.5	WASTE MANAGEMENT
8.6	SIDE-EFFECTS DETECTION
0.0	
8.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
0.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
88	REACTIVITY TOWARDS CONTAINER MATERIAL

9. References ld 26140-60-3
Date 23.07.2003

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(16)	Solutia Study no. XX-88-9289. Fate Testing For Therminol Biodegradation.
(17)	Solutia Study no. XX-84-X107; Acute Toxicity of Therminol 75 to Fathead Minnows.
(18)	Solutia Study no. AB-79-318B. Acute Toxicity of Therminol 88 to Rainbow Trout.
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(21)	Solutia Study No. AB-79 -317. Acute Toxicity of THERMINOL 88 to Daphnia magna.
(22)	Solutia Study No. BN-79-316. Toxicity of THERMINOL 88 to Freshwater Alga Selenastrum capricornutum.

# 9. References ld 26140-60-3 Date 23.07.2003

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(29)	Solutia Study No. BO-77-327; Mutagenicity Evaluation of CP 75052.
(30)	Solutia Study No. BO-77-328. Mutagenicity evaluation of CP 2321 SR.
(31)	Solutia Study no. PK-84-149. 1984. CHO/HGPRT Mammalian Cell Forward Gene Mutation Assay: THERMINOL 75.
(32)	Solutia Study no. PK-86-411. 1986. CHO/HGPRT Mammalian Cell Forward Gene Mutation Assay: SANTOWAX R.
(33)	Solutia Study No. SR-84-414; An Assessment of the Mutagenic Potential of THERMINOL

# 10. Summary and Evaluation

ld 26140-60-3 **Date** 23.07.2003

10.1	<b>FND</b>	<b>POINT</b>	·SI	JMM	ARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

# IUCLID

# **Data Set**

 Existing Chemical
 : ID: 92-06-8

 CAS No.
 : 92-06-8

 Common name
 : meta-terphenyl

 TSCA Name
 : m-terphenyl

 EINECS Name
 : m-terphenyl

 EC No.
 : 202-122-1

 Molecular Formula
 : C18H14

Producer related part

Company : Solutia Inc. Creation date : 17.03.2003

Substance related part

Company : Solutia Inc. Creation date : 17.03.2003

Status : Memo :

Printing date : 23.07.2003

Revision date :

Date of last update : 09.07.2003

Number of pages : 23

**Chapter (profile)** : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 **Reliability (profile)** : Reliability: without reliability, 1, 2, 3, 4

Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),

Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

# 1. General Information

ld 92-06-8 **Date** 23.07.2003

1.0.1	APPLICANT AND COMPANY INFORMATION
1.0.2	LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR
400	IDENTITY OF DECIDIENTS
1.0.3	IDENTITY OF RECIPIENTS
1.0.4	DETAILS ON CATEGORY/TEMPLATE
1.1.0	SUBSTANCE IDENTIFICATION
1.1.1	GENERAL SUBSTANCE INFORMATION
1.1.2	SPECTRA
1.2	SYNONYMS AND TRADENAMES
1.3	IMPURITIES
1.4	ADDITIVES
1.5	TOTAL QUANTITY
1.6.1	LABELLING
1.6.2	CLASSIFICATION
1.6.3	PACKAGING
11010	
1.7	USE PATTERN
1.7.1	DETAILED USE PATTERN
1.7.2	METHODS OF MANUFACTURE

# 1. General Information

ld 92-06-8 **Date** 23.07.2003

1.8	REGULATORY MEASURES
1.8.1	OCCUPATIONAL EXPOSURE LIMIT VALUES
1.8.2	2 ACCEPTABLE RESIDUES LEVELS
1.8.3	B WATER POLLUTION
1.8.4	MAJOR ACCIDENT HAZARDS
1.8.5	5 AIR POLLUTION
1.8.6	LISTINGS E.G. CHEMICAL INVENTORIES
1.9.1	DEGRADATION/TRANSFORMATION PRODUCTS
1.9.2	2 COMPONENTS
1.10	SOURCE OF EXPOSURE
1.11	ADDITIONAL REMARKS
1.12	LAST LITERATURE SEARCH
1.13	REVIEWS

ld 92-06-8 **Date** 23.07.2003

### 2.1 MELTING POINT

Value :  $= 87 - ^{\circ}C$ 

Sublimation

Method : other: not reported

Year

GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : CRC Handbook; SRC PhysProp Database

**Test substance**: m-Terphenyl [CAS No. 92-06-8]

**Reliability** : (2) valid with restrictions

19.06.2003 (1) (2)

### 2.2 BOILING POINT

Value :  $= 363 - ^{\circ}C$  at

Decomposition

Method : other: not reported

Year :

GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : CRC Handbook; SRC PhysProp Database

**Test substance** : m-Terphenyl [CAS No. 92-06-8] **Reliability** : (2) valid with restrictions

19.06.2003 (1) (2)

### 2.3 DENSITY

### 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

**Value** : = .0000233 - hPa at 25 °C

Decomposition

**Method** : other (measured): not reported

Year

**GLP** : no data **Test substance** : other TS

Remark : Reported as 1.75 x 10e-5 mm Hg @ 25 deg. C.

Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : Daubert and Danner. 1992
Test substance : m-Terphenyl [CAS No. 92-06-8]

**Reliability** : (2) valid with restrictions

19.06.2003 (3)

ld 92-06-8 Date 23.07.2003

### 2.5 PARTITION COEFFICIENT

Partition coefficient octanol-water = 5.52 - at °C Log pow

pH value

Method other (calculated): atom/fragment contribution method

Year

**GLP** no Test substance other TS

Method Individual atom/fragment contribution (AFC) values were determined for

> 130 simple chemical substructures. Another 235 correction factors were determined for various substructure orientations. The partition coefficient (log P) of a compound is estimated by summing all AFC values and

correction factors for a given chemical structure.

Remark Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Meylan and Howard. 1995 Source Test substance m-Terphenyl [CAS No. 92-06-8] Reliability (2) valid with restrictions

09.07.2003 (4)

### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in Water

Value = 1.51 - mg/l at 25 °C

pH value

concentration at °C

Temperature effects

Examine different pol.

at 25 °C pKa

Description slightly soluble (0.1-100 mg/L)

Stable

Deg. product

Method other: measured, method not reported

Year

**GLP** : no data Test substance other TS

Remark Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source Yalkowsky and Dannenfelser. 1992. Test substance m-Terphenyl [CAS No. 92-06-8]

Reliability (2) valid with restrictions

19.06.2003 (5)

Solubility in Water

Value .11 - at 25 °C

Ha value at °C concentration

**Temperature effects** Examine different pol.

pKa at 25 °C

Description

Stable

Deg. product

Method other Year 1984 **GLP** : no

5/23

ld 92-06-8 **Date** 23.07.2003

**Test substance**: other TS

**Method** : Estimation of aqueous solubility was based on plotting the aqueous

solubility vs the corrected retention time for calibration compounds. The estimation fit the following equation: log (RT)=-0.1946 log (uS)+1.091 with a linear correlation coefficient = 0.995, where RT=corrected retention time using reverse phase liquid chromatography and uS-aqueous solubility in u

moles/L.

A parallel estimation of water solubility used the method of Yalkowsky and Valvani (J.Chem. Eng. Data 24:127, 1979) which provided a correlation between aqueous solubility and octanol/water partition coefficient

development.

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

**Result** : Estimation of the aqueous solubility using the Calibration Curve method

was 0.11 ppm while estimation of correlation with the Kow derived an

estimate of 0.67 ppm.

**Test substance** : m-Terphenyl

**Reliability** : (2) valid with restrictions

19.06.2003 (6)

### 2.6.2 SURFACE TENSION

### 2.7 FLASH POINT

### 2.8 AUTO FLAMMABILITY

### 2.9 FLAMMABILITY

### 2.10 EXPLOSIVE PROPERTIES

### 2.11 OXIDIZING PROPERTIES

### 2.12 DISSOCIATION CONSTANT

### 2.13 VISCOSITY

### 2.14 ADDITIONAL REMARKS

ld 92-06-8 **Date** 23.07.2003

### 3.1.1 PHOTODEGRADATION

Type : water
Light source : Sun light
Light spectrum : - nm

**Relative intensity** : - based on intensity of sunlight

DIRECT PHOTOLYSIS

Halflife t1/2 : = 140 - day(s)

**Degradation** : 14 - % after 29 day(s)

Quantum yield
Deg. product

**Method** : other (measured)

Year : 1983 GLP : no Test substance : other TS

Method : A 20 ppm solution of m-terphenyl was prepared in a 50:50 mixture of

deionized water and acetonitrile. The solutions were then poured into a series of quartz tubes which were placed in sunlight. Duplicate tubes were prepared but wrapped in aluminum foil to serve as a dark control. One light-exposed and one dark-control sample were analyzed on days 0, 1, 3, 7, 14 and 29. Weather conditions were generally sunny with daytime temp.

reaching 90-95 deg. F. throughout the study. Sample preparation consisted of decanting 5 ml of the solution into a 15 ml centrifuge tube to which was added 3 g of NaCl to saturate the solution and separate acetonitrile from water. Isooctane (5 ml) was pipetted into the centrifuge tube and the mixture shaken vigorously for 2 min. One ml of isooctane was withdrawn and added to a GC autosampler vial. Anthracene was added as an internal standard. Extracts were analyzed by capillary GC using a flame

ionization detector. Triplicate extracts were analyzed at 20 ppm and a

single extraction at 2 ppm.

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Result : A half-life of 140 day was calculated. Approximately a 14% decrease in

concentration was observed after 29 days of sunlight exposure. The %age of test material remaining (in parentheses) after days of exposure in sunlight:dark control were: day 0 (100%), day 1 (105/108%), day 3 (98/96%), day 7 (86/96%), day 14 (103/113%) and day 29 (76/88%). The absorbance of a 20 ppm acetonitrile:water (50:50) solution of m-Terphenyl

at 290 nm was 0.24/cm pathlength.

**Test substance** : Meta-Terphenyl from Monsanto Chemicals procurement lab; purity

unspecified.

**Reliability** : (2) valid with restrictions

19.06.2003 (7)

Type : other Light source :

**Light spectrum** : - nm

Relative intensity : - based on intensity of sunlight

Deg. product

Method : other (calculated): AOPWIN v1.90

Year :

GLP : no
Test substance : other TS

**Remark**: Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Vapor phase m-terphenyl is susceptible to reaction with photochemically produced hydroxyl (OH) radicals. The 2nd order rate constant for reaction

ld 92-06-8 **Date** 23.07.2003

with hydroxyl radicals was calculated as 12.66E-12 cm3/(molecule\*sec). Based on 1.5E6 OH molecules/cm3 and assuming 12 hours of sunlight per

day, the estimated photo-oxidation half-life is 20.3 hours.

Source : EPIWIN

**Test substance** : m-Terphenyl [CAS No. 92-06-8] **Reliability** : (2) valid with restrictions

19.06.2003 (8)

### 3.1.2 STABILITY IN WATER

**Remark**: The test substance (m-Terphenyl) is not susceptible to hydrolysis.

13.05.2003

### 3.1.3 STABILITY IN SOIL

### 3.2.1 MONITORING DATA

### 3.2.2 FIELD STUDIES

### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III

Media: other: air-water-soil-sedimentAir: .87 % (Fugacity Model Level I)Water: 11.8 % (Fugacity Model Level I)Soil: 45 % (Fugacity Model Level I)Biota: % (Fugacity Model Level II/III)Soil: 42.4 % (Fugacity Model Level II/III)

Method : other Year : 2003

Method : Used EPIWIN (Syracuse Research Corp., Syracuse, NY). Physical

properties of m-terphenyl used as the model input parameters were: water solubility = 1.51 mg/L, vapor pressure = 1.75E-5 Hg; log Kow = 5.52; melting point = 87 deg. C. All property values were taken from this Robust

Summary.

**Remark** : Air: half life = 20.3 hr; emissions = 1000 kg/hr

Water: half life = 900 hr; emissions = 1000 kg/hr Soil: half life = 900 hr, emissions = 1000 kg/hr Sediment: half life = 3600 hr; emissions = 1000 kg/hr

Persistence Time: 972 hr

Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

**Test substance** : m-Terphenyl

**Reliability** : (2) valid with restrictions

19.06.2003

### 3.3.2 DISTRIBUTION

ld 92-06-8 **Date** 23.07.2003

### 3.4 MODE OF DEGRADATION IN ACTUAL USE

### 3.5 BIODEGRADATION

Type : aerobic inoculum : other

**Concentration** : 20 mg/l related to Test substance

related to

Contact time : 55 day(s)

**Degradation** : 38 - (±) % after 55 day(s)

Result : Deg. product :

 Method
 : other

 Year
 : 1983

 GLP
 : no

 Test substance
 : other TS

Method : Ultimate biodegradation screening study using a shake flask carbon

dioxide procedure carried out over a 55-day period. Testing used a commercially available inoculum purported to be specifically adapted to hydrocarbons. The test material was exposed to a microbial population with a plate count of 1.3x10E8 colony-forming units/ml in an aqueous inorganic salts medium. The BOD medium employed contained twice the standard level of phosphate buffer, four times the level of ferric chloride, the standard amount of calcium chloride and magnesium sulfate and 40 mg (NH4)2 SO4 per liter of water. One L of medium was charged to a 2-L Erlenmeyer flask and sparged with 70% oxygen in nitrogen.A 10 mL aliquot of settled supernatant from the blending operation for medium preparation was added to each test flask as the inoculum. After inoculum addition, 20 mg test chemical was added and triplicate flasks prepared. Each flask contained a reservoir holding barium hydroxide for capture and

quantification of CO2 level. After sealing all flasks were agitated on a rotary shaker in the dark at ambient temperature until analyzed after 55 days on test. Analysis of the barium hydroxide solutions was performed using a Fisher Automated Titration system. The per cent carbon was calculated from molecular parameters. Glucose served as the reference chemical to

verify methodology.

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Result : Following 55 days of exposure, a mean (3 reps) level of 38% (SD = 18)

with range of 19-53% CO2 evolution was achieved.

**Test substance**: Sample of m-Terphenyl obtained from Monsanto Co. Chemical

Procurement Laboaratory with confirmed GC purity of >95%.

**Reliability** : (2) valid with restrictions

19.06.2003 (9)

Type : aerobic

inoculum : other: Mississippi River Water

Contact time

**Degradation** : 100 - (±) % after 28 day(s)

**Result**: other: Biodegradable after long acclimation period

Deg. product

Method : other: River Die Away Test

Year : 1983 GLP : no Test substance : other TS

**Method** : Samples of Mississippi River water (suspended solids= 51 mg/L; pH =

8.25; microbial colonies/ml = 5.5x10E4), were allowed to settle for 2 days and then decanted through glass wool. Thereafter, 500 ml aliquots were

9/23

ld 92-06-8 **Date** 23.07.2003

and then decanted through glass wool. Thereafter, 500 ml aliquots were placed in glass testing vessels. Each test jar was spiked with 50 ppb test material in methylene chloride, the jars sealed and stored at ambient temperature in the dark until sampled. One jar of test material and 1 jar of sterilized control water were sampled on test days 0, 1, 3, 7, 16, and 28. Bottles were extracted 3x with methylene chloride, the solvent condensed and analyzed using GC/FID. Analytical methodology had been verified for accuracy prior to study start. A second trial was conducted with another sample of Mississippi River water whe reby each of the three Terphenyl isomers, ortho, meta and para, were added as a mixture at a rate of 20 ppb each. Similar procedures were followed for incubation and analysis, with one exception, this study was extended to 42 days for the final analysis.

**Remark** : Supplemental information which supports the conclusion that m-Terphenyl

is capable of biological degradation in the environment.

Result : After a relatively long (16-day) acclimation period, m-Terphenyl rapidly

degraded (complete degradation by test day 28) during both the first and

second trial.

Test substance : meta-Terphenyl, obtained from the Monsanto Procurement Laboratory,

with GC-confirmed purity > 95%. Samples of the other two Terphenyl isomers used in the Mixture trial also were verified as > 95% pure.

Reliability : (2) valid with restrictions

19.06.2003 (10)

## 3.6 BOD5, COD OR BOD5/COD RATIO

## 3.7 BIOACCUMULATION

## 3.8 ADDITIONAL REMARKS

4. Ecotoxicity ld 92-06-8

Pate 23.07.2003

#### 4.1 ACUTE/PROLONGED TOXICITY TO FISH

Туре

 Species
 : other: fish

 Exposure period
 : 96 hour(s)

 Unit
 : mg/l

 LC50
 : = .084

**Method** : other: calculated (EcoSAR)

Year

GLP : no Test substance : other TS

Method : An acute fish 96-h LC50 was calculated using ECOSAR, from the USEPA.

The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within

ECOSAR.

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

**Test substance**: m-Terphenyl [CAS No. 92-06-8]

13.05.2003 (11)

## 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static

Species : Daphnia magna (Crustacea)

**Exposure period** 48 hour(s) Unit mg/l **NOEC** >= .011 -EC50 = .022 -**Analytical monitoring** Method : other Year 1983 : **GLP** : yes : other TS Test substance

Remark

Method : Used EPA method (1975) 660/3-75-009 Committee on Methods for Acute

Toxicity Tests with Fish, Macroinvertebrates and Amphibians. Ten <24-h old D. magna Straus were selected from an in-house colony and tested at an ave. temp. of 21.2 deg. C in a series of three replicates per test concentration. Test concentrations were 0.011, 0.018, 0.03, 0.05 and 0.083 mg/L, plus clean water and solvent (dimethylformamide) controls. Tests were conducted in capped test vessels to preclude volatilization and used well water from St. Peters, Mo. Concentrations were not measured. Daphnids were not fed. Tests were conducted in 8 oz. glass beakers containing 200 mL of solution. Water quality was measured for Dissolved Oxygen, pH, alkalinity, water hardness, and temperature. No significant change were observed in any parameter measured. LC50 and CI were calculated using EPA statistical procedures.

: Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

**Result** : 48-h EC50 (95% CL) = 0.022 mg/L (0.019-0.025 mg/L). NOEC = 0.011

mg/L. % immobility (in parenthesis) seen after 24-h: control (0), solvent control (3), 0.011 mg/L (0), 0.018 mg/L (10), 0.03 mg/L (13), 0.05 mg/L (7), and 0.083 mg/L (37); and at 48-hr: control (0), solvent control (3), 0.011 mg/L (7), 0.018 mg/L (37), 0.03 mg/L (73), 0.05 mg/L (93), and 0.083 mg/L (100). pH ranged from 7.8 -8.2; DO ranged from 6.0-8.3; alkalinity ranged from 186-204 mg/L CaCO3; hardness ranged from 180-198 mg/L CaCO3.

4. Ecotoxicity ld 92-06-8

Pate 23.07.2003

**Test substance** : Analytical grade sample of m-Terphenyl; purity unkown.

**Reliability** : (2) valid with restrictions

19.06.2003 (12)

Type

Species : Daphnia sp. (Crustacea)

 Exposure period
 : 48 hour(s)

 Unit
 : mg/l

 LC50
 : = .115 

**Method** : other: calculated (EcoSAR)

Year

GLP : no Test substance : other TS

Remark : An acute Daphnia 48-h LC50 was calculated using ECOSAR, from the

USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES

notations within ECOSAR.

Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Test substance : m-Terphenyl [CAS No. 92-06-8]

13.05.2003 (11)

## 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

**Species** : other algae: green algae

Endpoint

 Exposure period
 : 96 hour(s)

 Unit
 : mg/l

 LC50
 : = .088 

Method : other: calculated (EcoSAR)

Year

GLP : no Test substance : other TS

Method : An acute green algal 96-h LC50 was calculated using ECOSAR, from the

USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES

notations within ECOSAR.

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Test substance : m-Terphenyl [CAS No. 92-06-8]

13.05.2003 (11)

## 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

## 4.5.1 CHRONIC TOXICITY TO FISH

## 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

## 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

## 4. Ecotoxicity

4.6.2	TOXICITY	TO TERRESTRI	AL PLANTS
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- 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS
- 4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES
- 4.7 BIOLOGICAL EFFECTS MONITORING
- 4.8 BIOTRANSFORMATION AND KINETICS
- 4.9 ADDITIONAL REMARKS

5. Toxicity ld 92-06-8

Pate 23.07.2003

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

#### 5.1.1 ACUTE ORAL TOXICITY

Type : LD50

**Value** : = 2400 - mg/kg bw

Species : rat

Strain : Sprague-Dawley
Sex : male/female

Number of animals

Vehicle : other

Doses : 500-10,000 mg/kg
Method : other (calculated)

Year : 1962 GLP : no Test substance : other TS

Method : Method used consistent with OECD 401, but conducted prior to its

codification. Groups of 5 male and female SD rats were administered test material in logarithmetically spaced dosages between 500 and 10,000 mg/kg. Each dosage was given once by gavage as a 20% suspension in corn oil. Animals were observed for 14 days after which they were necropsied. LD50 and CI were calculated according to the method of Weil.

After determination of the LD50 additional groups of 5 rats were

administered the test article in a similar fashion at dosages of 1000, 2000 and 4000 mg/kg and observed for up to 14 days. During this period, checks on food consumption and body weight were made and obervation of clinical signs of toxicity recorded. Liver and kidney weights (and corresponding organ:body weight ratios) were calculated. Necopsies were performed and histopathological examinations were conducted on the following organs:

heart, liver, lung, adrenals, kidneys and spleen.

**Remark**: Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]. Study adequate to provide corroborative

information in assessment of Mixed Terphenyls.

**Result** : LD50=2,400 mg/kg (95% CL=1600-3700). At 1000 mg/kg, no deaths

occurred and only a short-term (1-2 day) weight loss was observed. Similar signs seen at 2000 mg/kg, although 2 deaths were reported. At 4000 mg/kg acute distress was observed within 3-5 hrs followed by vocalization upon touch; deaths occurred within 48 hrs. No histopathological effects were reported for any test group and liver and kidney weight ratios relative to

body weight were considered normal.

**Test substance**: Reagent grade meta-terphenyl, verified for purity but unspecified.

**Reliability** : (2) valid with restrictions

19.06.2003 (13)

## 5.1.2 ACUTE INHALATION TOXICITY

## 5.1.3 ACUTE DERMAL TOXICITY

## 5.1.4 ACUTE TOXICITY, OTHER ROUTES

ld 92-06-8 5. Toxicity Date 23.07.2003

#### 5.2.1 SKIN IRRITATION

## 5.2.2 EYE IRRITATION

#### 5.3 **SENSITIZATION**

#### 5.4 REPEATED DOSE TOXICITY

Type Sub-acute **Species** : rat Sex no data

Strain Sprague-Dawley

Route of admin. : oral feed Exposure period 30 days Frequency of treatm. daily Post exposure period none

**Doses** 500, 250 and 100 mg/kg body weight

Control group yes

NOAEL = 100 - mg/kg bw

Method other Year 1962 GLP no **Test substance** other TS

Method Groups of 5 SD rats (sex unspecified) were fed inhouse diet admixed with

either 100, 250 or 500 mg/kg/body wt. test material for 30 consecutive days. Water was available ad libitum. All rats underwent gross necropsy at the end of the study and liver and kidney weights recorded. Body weights were measured on test days 11, 21 and 28. Heart, liver, lungs, kidneys, adrenals and spleen were examined microscopically at all test levels

Result 100 mg/kg - Overall NOEL. At 250 mg/kg/d - Slight reduction in body

weight at the end of the study; Liver weight and ratio were statistically elevated; no discernable effects on kidney wt. or histopathology of any organ. At 500 mg/kg/d - A significant reduction in body weight was observed at the end of the study. Liver weight /ratio were statistically elevated but Kidney weight/ratio were normal. No histopathological effects

noted in organs examined.

Test substance Reagent grade meta-terphenyl purchased from Eastman Chemical and

confirmed for purity.

Reliability (2) valid with restrictions

> Provided as Supplemental information; this study provides additional subacute information of some reliance on one of the terphenyl isomers

found in Mixed Terphenyls.

13.05.2003 (13)

Type Sub-acute **Species** rat Sex male Strain Wistar Route of admin. : oral feed : 14 days Exposure period Frequency of treatm. : daily Post exposure period : none

Doses : 0.2 % in the diet (2000 ppm)

**Control group** : yes LOAEL = .2 - % 5. Toxicity ld 92-06-8

Date 23.07.2003

 Method
 : other

 Year
 : 1974

 GLP
 : no

 Test substance
 : other TS

Method : An unspecified number of young, adult male Wistar rats were administered

commercial diet containing 0.2% (2000 ppm) test material in corn oil (test material dissolved in diethyl ether) for 14 consecutive days. Food and water were provided ad libitum and recorded daily. Organs (liver, kidney, spleen, adrenal) were weighed at necrospy after 2 weeks on test. Blood was taken via heart puncture at the end of the study to assess plasma and liver cholesterol. Unspecified statistical methods used with p<0.05.

Result : After 14 days of testing, a significant (8%) reduction in body weight was

observed, along with a statistical increase (136%) in plasma cholesterol level, but not liver cholesterol. Food consumption was reduced statistically as were adrenal, kidney, liver and spleen weights. Liver hypertrophy was

reported.

**Test substance**: Meta-Terphenyl obtained from Wako Pure Chemical Co., Tokyo.

**Reliability** : (4) not assignable

Provided as Supplemental information.

13.05.2003 (14)

## 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** : Salmonella typhimurium reverse mutation assay

System of testing : TM 677

**Test concentration**: several concentrations up to the limit of solubility of 900 uM

Cycotoxic concentr.

Metabolic activation: withResult: negativeMethod: otherYear: 1979GLP: noTest substance: other TS

**Method** : Salmonella exposed to test material concentrations for 2 hr in the presence

of 10% postmitochondrial supernatant (obtained separately from

phenobarbital and Arochlor pretreated male SD rats) along with cofactors supporting metabolic activation. Bacteria were centrifuged, resuspended and plated under selective and nonselective conditions. Mutant colonies were counted after 48 hr growth at 37 deg. F and the ratio of mutations on selective vs nonselective media examined. Positive response was considered on basis of achieving a mutation fraction higher than the

99%CL of the mean background fraction.

Result : When tested up to the maximum level of solubility using both phenobarbital

and Arochlor S9 fractions, no evidence of mutagenic response was

observed.

**Test substance**: Sample of meta-Terphenyl obtained from Annalabs, Inc. North Haven,

Conn. Purity unspecified.

**Reliability** : (4) not assignable

Supplementary information provided on one isomeric component of Mixed

Terphenyls.

22.04.2003 (15)

### 5.6 GENETIC TOXICITY 'IN VIVO'

5. Toxicity ld 92-06-8

Pate 23.07.2003

### 5.7 CARCINOGENICITY

#### 5.8.1 TOXICITY TO FERTILITY

## 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

## 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Type : other In vitro : In vitro Species : mouse Sex : male/female Strain : other

Route of admin. : other

**Exposure period** : 20-24 hr incubation

Frequency of treatm. : once

Duration of test

**Doses** : 0, 0.1, 1, 10 ug/mL.

Control group : other

Result : Statistical decrease in IVF & increased abnormal embryos and

degenerative oocytes at 1 and 10 ug/mL.

Method: otherYear: 1994GLP: noTest substance: other TS

Method : Used the mouse in vitro fertilization (IVF) technique to measure effects on

fertilization and early embryo development. Male and female mice from inhouse-bred strain B6D2F1 young adults were used. Food and water were provided ad libitum while light cycle and temperature were controled. Female mice were superovulated by IP injection of 10 IU of serum gonadotropin followed by 10 IU human chorionic gonadotropin (HCG). 12-15 hrs after addition of HCG, sperm was collected from the cauda epididymides from adult male mice. After verification of sperm viability and motility, oocytes were recovered from superovulated mice and exposed to 2-3 million sperm in an incubation medium containing test material for 20-24 hrs. Test substance was suspended in BMOC-3 culture medium with minimal alcohol (0.01%) and then mixed with medium to attain dosages of 0.1, 1 or 10 ug/mL test substance. Each culture dish containing test material, sperm and oocytes was scored for fertilized or degenerative

oocytes and abnormal embryos. Fertilization was considered to have occurred in the presence of 1 cell with 2 pronuclei, 2 cells with 1 polar body or a 2-celled embryo. Three-to-5 trials were conducted per test

concentration. Mean scores were statistically evaluated using Chi Square and Bonferroni Chi Square Contingency Tables with p<0.05.

Remark
Result
Supplemental information; study inadequate to support this HPV endpoint.
No treatment-related effects were observed at 0.1 ug/mL A statistically

significant decrease in FIV and increases in abnormal embryos and degererative oocytes were observed at 1 and 10 ug/mL

**Test substance**: Purchased from AccuStandard, Inc. CT and verified by GC-FID as 99%

pure m-terphenyl.

Reliability : (3) invalid

19.06.2003 (16)

# 5. Toxicity ld 92-06-8 Date 23.07.2003

59	SPECIFIC	

## 5.10 EXPOSURE EXPERIENCE

## 5.11 ADDITIONAL REMARKS

## 6. Analyt. Meth. for Detection and Identification

- 6.1 ANALYTICAL METHODS
- 6.2 DETECTION AND IDENTIFICATION

# 7. Eff. Against Target Org. and Intended Uses

7.1	FUNCTION
7.2	EFFECTS ON ORGANISMS TO BE CONTROLLED
7.3	ORGANISMS TO BE PROTECTED
7.0	ONORMONO TO BET NOTESTED
7.4	USER
7.5	RESISTANCE

# 8. Meas. Nec. to Prot. Man, Animals, Environment

8.1	METHODS HANDLING AND STORING
8.2	FIRE GUIDANCE
8.3	EMERGENCY MEASURES
8.4	POSSIB. OF RENDERING SUBST. HARMLESS
8.5	WASTE MANAGEMENT
8.6	SIDE-EFFECTS DETECTION
O.O	
8.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
0.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
8.8	REACTIVITY TOWARDS CONTAINER MATERIAL

# 9. References ld 92-06-8 Pate 23.07.2003

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# 10. Summary and Evaluation

ld 92-06-8 **Date** 23.07.2003

10.1 END POINT SUMM	AKY
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10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

# IUCLID

# **Data Set**

**Existing Chemical** : ID: 84-15-1 **CAS No.** : 84-15-1

TSCA Name : ortho-Terphenyl

Producer related part

Company : Solutia Inc. Creation date : 17.03.2003

Substance related part

Company : Solutia Inc. Creation date : 17.03.2003

Status : Memo :

Printing date : 23.07.2003

Revision date

Date of last update : 23.07.2003

Number of pages : 25

**Chapter (profile)**: Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)
: Reliability: without reliability, 1, 2, 3, 4

Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TALuft (DE),

Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1. General Information

1.0.1	APPLICANT AND COMPANY INFORMATION
1.0.2	LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR
1.0.3	IDENTITY OF RECIPIENTS
1.0.4	DETAILS ON CATEGORY/TEMPLATE
1.1.0	SUBSTANCE IDENTIFICATION
1.1.1	GENERAL SUBSTANCE INFORMATION
1.1.2	SPECTRA
1.2	SYNONYMS AND TRADENAMES
1.3	IMPURITIES
1.4	ADDITIVES
1.5	TOTAL QUANTITY
1.6.1	LABELLING
1.6.2	CLASSIFICATION
1.6.3	PACKAGING
1.7	USE PATTERN
1.7.1	DETAILED USE PATTERN
1.7.2	METHODS OF MANUFACTURE

## 1. General Information

1.8	REGULATORY MEASURES
1.8.1	OCCUPATIONAL EXPOSURE LIMIT VALUES
1.8.2	ACCEPTABLE RESIDUES LEVELS
1.8.3	WATER POLLUTION
1.8.4	MAJOR ACCIDENT HAZARDS
1.0.4	WIAJON ACCIDENT HAZANDS
1.8.5	AIR POLLUTION
1.8.6	LISTINGS E.G. CHEMICAL INVENTORIES
1.9.1	DEGRADATION/TRANSFORMATION PRODUCTS
1.9.2	COMPONENTS
1.10	SOURCE OF EXPOSURE
1.11	ADDITIONAL REMARKS
1.11	ADDITIONAL INLIGATION
1.12	LAST LITERATURE SEARCH
1.13	REVIEWS

ld 84-15-1 **Date** 23.07.2003

## 2.1 MELTING POINT

**Value** :  $= 56.2 - {}^{\circ}\text{C}$ 

Sublimation

Method : other: not reported

Year

GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : CRC Handbook; SRC PhysProp Database

Test substance : o-Terphenyl [CAS No. 84-15-1]
Reliability : (2) valid with restrictions

19.06.2003 (1) (2)

## 2.2 BOILING POINT

Value :  $= 332 - ^{\circ}C$  at

Decomposition

Method : other: not reported

Year :

GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : CRC Handbook; SRC PhysProp Database

Test substance : o-Terphenyl [CAS No. 84-15-1]
Reliability : (2) valid with restrictions

19.06.2003 (1) (2)

#### 2.3 DENSITY

## 2.3.1 GRANULOMETRY

## 2.4 VAPOUR PRESSURE

**Value** : = .0003 - hPa at 25 °C

Decomposition

**Method** : other (measured): not reported

Year

GLP : no data Test substance : other TS

Remark : Reported as 0.00025 mm Hg @ 25 deg. C.

Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : Daubert and Danner. 1989
Test substance : o-Terphenyl [CAS No. 84-15-1]
Reliability : (2) valid with restrictions

19.06.2003 (3)

ld 84-15-1 **Date** 23.07.2003

### 2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water Log pow : = 5.28 - at °C

pH value : -

Method : other (measured): not reported

Year

GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : Ogata et al. 1984

Test substance : o-Terphenyl [CAS No. 84-15-1]
Reliability : (2) valid with restrictions

19.06.2003 (4)

Partition coefficient : octanol-water Log pow : = 5.52 - at °C

pH value : -

Method : other (calculated): atom/fragment contribution method

Year :

GLP : no Test substance : other TS

Method : Individual atom/fragment contribution (AFC) values were determined for

130 simple chemical substructures. Another 235 correction factors were determined for various substructure orientations. The partition coefficient (log P) of a compound is estimated by summing all AFC values and

correction factors for a given chemical structure.

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : Meylan and Howard. 199
Test substance : o-Terphenyl [CAS No. 84-15-1]
Reliability : (2) valid with restrictions

19.06.2003 (5)

#### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water

**Value** : = 1.24 - mg/l at 25 °C

pH value : -

concentration : at °C

Temperature effects

Examine different pol.

**pKa** : at 25 °C

**Description** : slightly soluble (0.1-100 mg/L)

Stable

Deg. product

**Method** : other: measured, method not reported

Year

GLP : no data
Test substance : other TS

Remark : Supplemental Information Provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : Yalkowsky and Dannenfelser. 1992
Test substance : o-Terphenyl [CAS No. 84-15-1]

**Reliability** : (2) valid with restrictions

2.12 DISSOCIATION CONSTANT

ld 84-15-1 **Date** 23.07.2003

19.06.2003 (6)Solubility in : Water .83 - at 25 °C Value pH value concentration at °C Temperature effects Examine different pol. рKа at 25 °C Description **Stable** Deg. product Method other Year 1983 GLP no Test substance other TS Method Estimation of aqueous solubility was based on plotting the aqueous solubility vs the corrected retention time for calibration compounds. The estimation fit the following equation: log (RT)=-0.1946 log (uS)+1.091 with a linear correlation coefficient = 0.995, where RT=corrected retention time using reverse phase liquid chromatography and uS-aqueous solubility in u moles/L. A parallel estimation of water solubility used the method of Yalkowsky and Valvani (J.Chem. Eng. Data 24:127, 1979) which provided a correlation between aqueous solubility and octanol/water partition coefficient development. Remark Supplemental Information Provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3] Result Estimation of the aqueous solubility using the Calibration Curve method was 0.83 ppm while estimation of correlation with the Kow derived an estimate of 5.5 ppm. Test substance : o-Terphenyl Reliability (2) valid with restrictions 19.06.2003 (7)2.6.2 SURFACE TENSION 2.7 **FLASH POINT** 2.8 **AUTO FLAMMABILITY FLAMMABILITY** 2.9 **EXPLOSIVE PROPERTIES** 2.11 **OXIDIZING PROPERTIES** 

ld 84-15-1 **Date** 23.07.2003

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

ld 84-15-1 **Date** 23.07.2003

## 3.1.1 PHOTODEGRADATION

Type : water
Light source : Sun light
Light spectrum : - nm

Relative intensity : - based on intensity of sunlight

DIRECT PHOTOLYSIS

Halflife t1/2 :

**Degradation** : < 8 - % after 29 day(s)

Quantum yield
Deg. product

**Method** : other (measured)

Year : 1983 GLP : no Test substance : other TS

Method: A 20 ppm solution of o-terphenyl was prepared in a 50:50 mixture of

deionized water and acetonitrile. The solutions were then poured into a series of quartz tubes which were placed in sunlight. Duplicate tubes were prepared but wrapped in aluminum foil to serve as a dark control. One light-exposed and one dark-control sample were analyzed on days 0, 1, 3, 7, 14 and 29. Weather conditions were generally sunny with daytime temp.

reaching 90-95 deg. F. throughout the study. Sample preparation consisted of decanting 5 ml of the solution into a 15 ml centrifuge tube to which was added 3 g of NaCl to saturate the solution and separate acetonitrile from water. Isooctane (5 ml) was pipetted into the centrifuge tube and the mixture shaken vigorously for 2 min. One ml of isooctane was withdrawn and added to a GC autosampler vial. Anthracene was added as an internal standard. Extracts were analyzed by capillary GC using a flame

ionization detector. Triplicate extracts were analyzed at 20 ppm and a

single extraction at 2 ppm.

Remark : Supplemental Information Provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

**Result**: No significant decrease in concentration was observed after 29 days of

s unlight exposure. The %age of test material remaining (in parentheses) after days of exposure in sunlight/dark control were: day 0 (100%), day 1 (86/96%), day 3 (93/95%), day 7 (95/89%), day 14 (95/98%) and day 29 (92/91%). The absorbance of a 20 ppm acetonitrile:water (50:50) solution

of o-Terphenyl at 290 nm was 0.13/cm pathlength.

Test substance : Ortho-Terphenyl from Monsanto Chemicals procurement lab; purity

unspecified.

**Reliability** : (2) valid with restrictions

19.06.2003 (8)

Type : other Light source :

**Light spectrum** : - nm

Relative intensity : - based on intensity of sunlight

Deg. product

Method : other (calculated): AOPWIN v1.90

Year :

GLP : no Test substance : other TS

Remark : Supplemental Information Provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Vapor phase o -terphenyl is susceptible to reaction with photochemically produced hydroxyl (OH) radicals. The 2nd order rate constant for reaction with hydroxyl radicals was calculated as 9.1946E-12 cm3/(molecule\*sec). Based on 1.5E6 OH molecules/cm3 and assuming 12 hours of sunlight per

8/25

ld 84-15-1 **Date** 23.07.2003

Based on 1.5E6 OH molecules/cm3 and assuming 12 hours of sunlight per

day, the estimated photo-oxidation half-life is 27.9 hours.

Source : EPIWIN

Test substance : o-Terphenyl [CAS No. 84-15-1]
Reliability : (2) valid with restrictions

19.06.2003 (9)

## 3.1.2 STABILITY IN WATER

**Remark**: Test substance (o-Terphenyl) is not susceptible to hydrolysis.

13.05.2003

## 3.1.3 STABILITY IN SOIL

## 3.2.1 MONITORING DATA

#### 3.2.2 FIELD STUDIES

## 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III

Media: other: air-water-soil-sedimentAir: 1.29 % (Fugacity Model Level I)Water: 14.7 % (Fugacity Model Level I)Soil: 50.9 % (Fugacity Model Level I)Biota: % (Fugacity Model Level II/III)Soil: 33 % (Fugacity Model Level II/III)

Method : other Year : 2003

Method : Used EPIWIN (Syracuse Research Corp., Syracuse, NY). Physical

properties of o-terphenyl used as the model input parameters were water solubility of 1.24 mg/L; vapor pressure of 0.00025 mm Hg; log Kow of 5.28, and melting point of 56.2 deg. C. All property values were taken from this

Robust Summary.

**Remark** : Air: half life = 27.9 hr; emissions = 1000 kg/hr

Water: half life = 900 hr; emissions = 1000 kg/hr Soil: half life = 900 hr; emissions = 1000 kg/hr Sediment: half life = 3600 hr; emissions = 0 kg/hr

Persistence Time: 853 hr.

Supplemental Information Provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

**Reliability** : (2) valid with restrictions

09.07.2003

## 3.3.2 DISTRIBUTION

## 3.4 MODE OF DEGRADATION IN ACTUAL USE

ld 84-15-1 **Date** 23.07.2003

### 3.5 BIODEGRADATION

Type : aerobic Inoculum : other

**Concentration**: related to Test substance

related to

Contact time : 55 day(s)

**Degradation** :  $= 20 - (\pm 34) \%$  after 55 day(s)

Result

Deg. product : Method :

 Method
 : other

 Year
 : 1983

 GLP
 : no

 Test substance
 : other TS

Method : Ultimate biodegradaton screening study using a shake flask carbon dioxide

procedure carried out over a 55-day period. Testing used a commercially available inoculum purported to be specifically adapted to hydrocarbons. The test material was exposed to a microbial population with a plate count of 1.3x10E8 colony-forming units/ml in an aqueous inorganic salts medium. The BOD medium employed contained twice the standard level of

phosphate buffer, four times the level of ferric chloride, the standard amount of calcium chloride and magnesium sulfate and 40 mg (NH4)2 SO4 per liter of water. One L of medium was charged to a 2-L Erlenmeyer flask and sparged with 70% oxygen in nitrogen. A 10 mL aliquot of settled supernatant from the blending operation for medium preparation was added to each test flask as the inoculum. After inoculum addition, 20 mg test chemical was added and triplicate flasks prepared. Each flask

quantification of CO2 level. After sealing all flasks were agitated on a rotary shaker in the dark at ambient temperature until analyzed after 55 days on test. Analysis of the barium hydroxide solutions was performed using a Fisher Automated Titration system. The per cent carbon was calculated from molecular parameters. Glucose served as the reference chemical to

contained a reservoir holding barium hydroxide for capture and

verify methodology.

**Remark**: Supplemental Information Provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

**Result** : Following 55 days of exposure, a mean (3 reps) level of 20% (SD = 34)

with range of 0-60% CO2 evolution was achieved.

**Test substance** : Sample of o -Terphenyl obtained from Monsanto Chemical Procurement

Laboaratory with confirmed GC purity of > 95%.

**Reliability** : (2) valid with restrictions

23.07.2003 (10)

Type : aerobic

Inoculum : other: Mississippi River Water

Contact time

**Degradation** :  $100 - (\pm) \%$  after 42 day(s)

**Result** : other: Biodegradable after long acclimation period

Deg. product

**Method** : other: River Die Away test

Year : 1983
GLP : no
Test substance : other TS

**Method** : Samples of Mississippi River water (suspended solids= 51 mg/L; pH =

8.25; microbial colonies/ml = 5.5x10E4), were allowed to settle for 2 days and then decanted through glass wool. Thereafter, 500 ml aliquots were placed in glass testing vessels. Each test jar was spiked with 50 ppb test material in methylene chloride, the jars sealed and stored at ambient temperature in the dark until sampled. One jar of test material and 1 jar of sterilized control water/were sampled on test days 0, 1, 3, 7, 16, and 28.

ld 84-15-1 **Date** 23.07.2003

sterilized control water were sampled on test days 0, 1, 3, 7, 16, and 28. Bottles were extracted 3x with methylene chloride, the solvent condensed and analyzed using GC/FID. Analytical methodology had been verified for accuracy prior to study start. A second trial was conducted with another sample of Mississippi River water whe reby each of the three Terphenyl isomers, ortho, meta and para, were added as a mixture at a rate of 20 ppb each. Similar procedures were followed for incubation and analysis, with one exception, this study was extended to 42 days for the final analysis.

**Remark** : Supplemental information which supports the conclusion that o-Terphenyl

is capable of biological degradation in the environment.

Result : After a long (28-day) acclimation period, o-Terphenyl rapidly degraded

(complete degradation by test day 42) during the second trial.

**Test substance** : ortho-Terphenyl, obtained from the Monsanto Procurement Laboratory,

with GC-confirmed purity > 95%. Samples of the other two Terphenyl isomers used in the Mixture trial also were verified as > 95% pure.

**Reliability** : (2) valid with restrictions

23.07.2003 (11)

## 3.6 BOD5, COD OR BOD5/COD RATIO

## 3.7 BIOACCUMULATION

## 3.8 ADDITIONAL REMARKS

4. Ecotoxicity ld 84-15-1

Pate 23.07.2003

#### 4.1 ACUTE/PROLONGED TOXICITY TO FISH

Туре

 Species
 : other: fish

 Exposure period
 : 96 hour(s)

 Unit
 : mg/l

 LC50
 : = .084

**Method** : other: calculated (EcoSAR)

Year

GLP : no Test substance : other TS

**Remark**: An acute fish 96-h LC50 was calculated using ECOSAR, from the USEPA.

The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within

ECOSAR.

Supplemental Information Provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

**Test substance** : o-Terphenyl [CAS No. 84-15-1]

19.06.2003 (12)

## 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static

Species : Daphnia magna (Crustacea)

**Exposure period** 48 hour(s) Unit mg/l **NOEC** >= .036 -EC50 = .045 -**Analytical monitoring** Method : other Year 1983 : **GLP** : yes : other TS Test substance

Method : Used EPA method (1975) 660/3-75-009 Committee on Methods for Acute

Toxicity Tests with Fish, Macroinvertebrates and Amphibians. Ten <24-h old D. magna Straus were selected from an in-house colony and tested at 20 +/-1 deg. C in a series of three replicates per test concentration. Test concentrations were 0.022, 0.036, 0.06, 0.1 and 0.167 mg/L, plus clean water and solvent (dimethylformamide) controls. Tests were conducted in capped test vessels to proclude volatilization and used well water from St. Peters, Mo. Concentrations were not measured. Daphnids were not fed. Tests were conducted in 8-oz. glass beakers containing 200 mL of solution. Water quality was measured for Dissolved Oxygen, pH, alkalinity, water hardness, and temperature. No significant change were observed in any parameter measured. LC50 and CI were calculated using EPA statistical procedures.

Remark : Supplemental Information Provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

**Result** : 48-h EC50 (95% CL) = 0.045 mg/L (0.036-0.060 mg/L). NOEC = 0.036

mg/L. % immobility (in parenthesis) seen after 24-h: control (0), solvent control (0), 0.022 mg/L (0), 0.036 mg/L (0), 0.06 mg/L (13), 0.1 mg/L (27), and 0.167 mg/L (60); and at 48-hr: control (0), solvent control (3), 0.022 mg/L (0), 0.036 mg/L (0), 0.06 mg/L (13), 0.1 mg/L (27), and 0.167 mg/L (60). pH ranged from 7.8-8.3; DO ranged from 7.5-8.4; alkalinity ranged from 186-206 mg/L CaCO3; hardness ranged from 180-194 mg/L CaCO3.

12/25

4. Ecotoxicity ld 84-15-1

Pate 23.07.2003

**Test substance** : Analytical grade sample o-Terphenyl; purity unkown.

**Reliability** : (2) valid with restrictions

13.05.2003 (13)

Type

Species : Daphnia sp. (Crustacea)

 Exposure period
 : 48 hour(s)

 Unit
 : mg/l

 LC50
 : = .115 

**Method** : other: calculated (EcoSAR)

Year

GLP : no Test substance : other TS

Remark : An acute Daphnia 48-h LC50 was calculated using ECOSAR, from the

USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES

notations within ECOSAR.

Supplemental Information Provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

**Test substance** : o-Terphenyl [CAS No. 84-15-1]

13.05.2003 (12)

## 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : other algae: green algae

Endpoint

 Exposure period
 : 96 hour(s)

 Unit
 : mg/l

 LC50
 : = .088 

Method : other: calculated (EcoSAR)

Year

GLP : no Test substance : other TS

Remark : An acute green algal 96-h LC50 was calculated using ECOSAR, from the

USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES

notations within ECOSAR.

Supplemental Information Provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Test substance : o-Terphenyl [CAS No. 84-15-1]

09.07.2003 (12)

## 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

## 4.5.1 CHRONIC TOXICITY TO FISH

## 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

## 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

# 4. Ecotoxicity

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- 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS
- 4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES
- 4.7 BIOLOGICAL EFFECTS MONITORING
- 4.8 BIOTRANSFORMATION AND KINETICS
- 4.9 ADDITIONAL REMARKS

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

#### 5.1.1 ACUTE ORAL TOXICITY

Type : LD50

**Value** : = 1900 - mg/kg bw

Species : rat

Strain : Sprague-Dawley
Sex : male/female

Number of animals

Vehicle : other

Doses : 500-10,000 mg/kg
Method : other (calculated)

Year : 1962 GLP : no Test substance : other TS

Method : Method used consistent with OECD 401, but conducted prior to its

codification. Groups of 5 male and female SD rats were administered test material in logarithmetically spaced dosages between 500 and 10,000 mg/kg. Each dosage was given once by gavage as a 20% suspension in corn oil. Animals were observed for 14 days after which they were necropsied. LD50 and CI were calculated according to the method of Weil.

After determination of the LD50 additional groups of 5 rats were

administered the test article in a similar fashion at dosages of 500, 1000 and 2000 mg/kg and observed for up to 14 days. During this period, checks on food consumption and body weight were made and obervation of clinical signs of toxicity recorded. Liver and kidney weights (and corresponding organ:body weight ratios) were calculated. Necopsies were performed and histopathological examinations were conducted on the following organs:

heart, liver, lung, adrenals, kidneys and spleen.

Remark : Study adequate to provide corroborative information in assessment of

mixed terphenyls. Provided as Supplemental information.

Result : LD50=1,900 mg/kg (1300-2800 mg/kg). Generalized signs of toxicity were

observed in most animals, including rough coat and diarrhea. At 2000 and 1000 mg/kg: Two deaths occurred at 2000 mg/kg within 4 days and 1 death at 1000 mg/kg during the same period; animals exhibited cataplectic behavior and vocalization when touched within 8 days of dosing. The liverand kidney-to-body weight ratios were normal at all dose levels. No effects

were observed at 500 mg/kg.

**Test substance**: Reagent grade ortho-terphenyl, with purity verified but unspecified.

**Reliability** : (2) valid with restrictions

19.06.2003 (14)

## 5.1.2 ACUTE INHALATION TOXICITY

## 5.1.3 ACUTE DERMAL TOXICITY

## 5.1.4 ACUTE TOXICITY, OTHER ROUTES

## 5.2.1 SKIN IRRITATION

#### 5.2.2 EYE IRRITATION

#### 5.3 SENSITIZATION

#### 5.4 REPEATED DOSE TOXICITY

Type : Sub-acute
Species : rat
Sex : no data

**Strain** : Sprague-Dawley

Route of admin. : oral feed Exposure period : 30 days Frequency of treatm. : daily Post exposure period : none

Doses : 500, 250 and 100 mg/kg/d body weight

Control group : yes

**NOAEL** : = 100 - mg/kg bw

 Method
 : other

 Year
 : 1962

 GLP
 : no

 Test substance
 : other TS

Method : Groups of 5 SD rats (sex unspecified) were fed inhouse diet admixed with

either 100, 250 or 500 mg/kg/body wt. test material for 30 consecutive days. Water was available ad libitum. All rats underwent gross necropsy at the end of the study and liver and kidney weights recorded. Body weights were measured on test days 11, 21 and 28. Heart, liver, lungs, kidneys, adrenals and spleen were examined microscopically at all test levels

Result : 100 mg/kg - Overall NOEL. AT 250 mg/kg/d - Slight reduction in body

weight at the end of the study; Liver weight/ratio and kidney weight/ratio were statistically elevated; no discernable effects on histopathology of any organ. At 500 mg/kg/d - A significant reduction in body weight with rats losing 10-15 gm from their initial group weight after the first 10 days of testing. After 30 days on test, lost weight had been regained but 30-day value was substantially below control value. The Liver weight /ratio and Kidney weight/ratio were statistically elevated at study's end. No

histopathological effects noted in organs examined.

**Test substance** : Reagent grade ortho-terphenyl purchased from Eastman Chemical and

confirmed for purity but unspecified.

**Reliability** : (2) valid with restrictions

Provided as Supplemental information; this study provides additional subacute information of some reliance on one of the terphenyl isomers

found in Mixed Terphenyls.

29.04.2003 (14)

Type Sub-acute **Species** Sex male Strain Wistar Route of admin. : oral feed **Exposure period** 14 days Frequency of treatm. : daily Post exposure period : none

**Doses** : 0.2% in the diet ( 2000 ppm)

 Control group
 : yes

 LOAEL
 : = .2 - %

 Method
 : other

 Year
 : 1974

 GLP
 : no

 Test substance
 : other TS

Method : An unspecified number of young, adult male Wistar rats were administered

commercial diet containing 0.2% (2000 ppm) test material in corn oil (test material dissolved in diethyl ether) for 14 consecutive days. Food and water were provided ad libitum and recorded daily. Organs (liver, kidney, spleen, adrenal) were weighed at necrospy after 2 weeks on test. Blood was taken via heart puncture at the end of the study to assess plasma and liver cholesterol. Unspecified statistical methods used with p<0.05.

**Result** : After 14 days of testing, a significant (15%) reduction in body weight was

observed, along with an increased plasma cholesterol level (121%). Food consumption was reduced statistically as were adrenal and kidney weights.

Adrenal hypertrophy was reported.

**Test substance** : Ortho-Terphenyl obtained from Wako Pure Chemical Co., Tokyo.

**Reliability** : (4) not assignable

Provided as Supplemental information.

13.05.2003 (15)

## 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** : Salmonella typhimurium reverse mutation assay

System of testing : TM677

**Test concentration**: several concentrations up to the limit of solubility of 900 uM

Cycotoxic concentr.

Metabolic activation: withResult: negativeMethod: otherYear: 1979GLP: noTest substance: other TS

Method : Salmonella exposed to test material concentrations for 2 hr in the presence

of 10% postmitochondrial supernatant (obtained separately from phenobarbital and Arochlor pretreated male SD rats) along with cofactors supporting metabolic activation. Bacteria were centrifuged, resuspended and plated under selective and nonselective conditions. Mutant colonies were counted after 48 hr growth at 37 deg. F and the ratio of mutations on selective vs nonselective media examined. Positive response was considered on basis of achieving a mutation fraction higher than the

99%CL of the mean background fraction.

Result : When tested up to the maximum level of solubility using both phenobarbital

and Arochlor S9 fractions, no evidence of mutagenic response was

observed.

**Test substance**: Sample of ortho-Terphenyl obtained from Annalabs, Inc. North Haven,

Conn. Purity unspecified.

**Reliability** : (4) not assignable

Supplementary information provided on one isomeric component of Mixed

Terphenyls.

22.04.2003 (16)

## 5.6 GENETIC TOXICITY 'IN VIVO'

### 5.7 CARCINOGENICITY

#### 5.8.1 TOXICITY TO FERTILITY

## 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

## 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Type : other
In vitro/in vivo : In vitro
Species : mouse
Sex : male/female
Strain : other

Strain : other Route of admin. : other

**Exposure period** : 20-24 hr incubation

Frequency of treatm. : once

Duration of test

**Doses** : 0, 0.1, 1, 10 ug/mL.

Control group : yes

**Result**: Increased number of abnormal embryos and degenerative oocytes at and

above 1 ug/mL.

 Method
 : other

 Year
 : 1994

 GLP
 : no

 Test substance
 : other TS

Method : Used the mouse in vitro fertilization (IVF) technique to measure effects on

fertilization and early embryo development. Male and female mice from inhouse-bred strain B6D2F1 young adults were used. Food and water were provided ad libitum while light cycle and temperature were controled. Female mice were superovulated by IP injection of 10 IU of serum gonadotropin followed by 10 IU human chorionic gonadotropin (HCG). 12-15 hrs after addition of HCG, sperm was collected from the cauda epididymides from adult male mice. After verification of sperm viability and motility, oocytes were recovered from superovulated mice and exposed to 2-3 million sperm in an incubation medium containing test material for 20-

2-3 million sperm in an incupation medium containing test material for 20-24 hrs. Test substance was suspended in BMOC-3 culture medium with minimal alcohol (0.01%) and then mixed with medium to attain dosages of 0.1, 1 or 10 ug/mL test substance. Each culture dish containing test material, sperm and oocytes was scored for fertilized or degenerative oocytes and abnormal embryos. Fertilization was considered to have occurred in the presence of 1 cell with 2 pronuclei, 2 cells with 1 polar body or a 2-celled embryo. Three-to-5 trials were conducted per test

concentration. Mean scores were statistically evaluated using Chi Square

and Bonferroni Chi Square Contingency Tables with p<0.05.

Remark : Supplemental information; study inadequate to support this HPV endpoint.
Result : Statistically decreased IVF and increased number of abnormal embryos and degenerative oocytes at and above 1 ug/mL

: Purchased from AccuStandard, Inc. CT and verified by GC-FID as 99%

pure ortho-Terphenyl

Reliability : (3) invalid

**Test substance** 

19.06.2003 (17)

5.9	CDECIEIC	INVFSTIGA'	
20 4	SPECIFIC	INVESTICA	I K NV.

## 5.10 EXPOSURE EXPERIENCE

## 5.11 ADDITIONAL REMARKS

## 6. Analyt. Meth. for Detection and Identification

- 6.1 ANALYTICAL METHODS
- 6.2 DETECTION AND IDENTIFICATION

# 7. Eff. Against Target Org. and Intended Uses

7.1	FUNCTION
7.2	EFFECTS ON ORGANISMS TO BE CONTROLLED
7.3	ORGANISMS TO BE PROTECTED
7.4	USER
7.5	RESISTANCE

# 8. Meas. Nec. to Prot. Man, Animals, Environment

8.1	METHODS HANDLING AND STORING
8.2	FIRE GUIDANCE
8.3	EMERGENCY MEASURES
8.4	POSSIB, OF RENDERING SUBST, HARMLESS
-	
8.5	WASTE MANAGEMENT
0.10	
8.6	SIDE-EFFECTS DETECTION
0.0	GDE ET EGTO DETEGTION
8.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
0.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
88	REACTIVITY TOWARDS CONTAINER MATERIAL
XX	REALTIVITY TOWARDS CONTAINER WATERIAL

# 9. References ld 84-15-1

Date 23.07.2003

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9. References

ld 84-15-1 **Date** 23.07.2003

# 10. Summary and Evaluation

ld 84-15-1 Date 23.07.2003

10.1	<b>FND</b>	POINT	SI	JMMARY	1

# 10.2 HAZARD SUMMARY

# 10.3 RISK ASSESSMENT

# IUCLID

# **Data Set**

Existing Chemical : ID: 92-94-4

CAS No. : 92-94-4

Common name : para-terphenyl

TSCA Name : p-Terphenyl

EINECS Name : p-terphenyl

EC No. : 202-205-2

Producer related part

Company : Solutia Inc.
Creation date : 17.03.2003

Substance related part

Company : Solutia Inc.
Creation date : 17.03.2003

Status : Memo :

Printing date : 23.07.2003

Revision date

Date of last update : 23.07.2003

Number of pages : 24

**Chapter (profile)** : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 **Reliability (profile)** : Reliability: without reliability, 1, 2, 3, 4

Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),

Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

# 1. General Information

1.0.1	APPLICANT AND COMPANY INFORMATION
1.0.2	LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR
1.0.3	IDENTITY OF RECIPIENTS
1.0.4	DETAILS ON CATEGORY/TEMPLATE
1.1.0	SUBSTANCE IDENTIFICATION
1.1.1	GENERAL SUBSTANCE INFORMATION
1.1.2	SPECTRA
1.2	SYNONYMS AND TRADENAMES
1.3	IMPURITIES
1.4	ADDITIVES
1.5	TOTAL QUANTITY
1.6.1	LABELLING
1.6.2	CLASSIFICATION
1.6.3	PACKAGING
1.7	USE PATTERN
1.7.1	DETAILED USE PATTERN
1.7.2	METHODS OF MANUFACTURE

# 1. General Information

1.8	REGULATORY MEASURES
1.8.1	OCCUPATIONAL EXPOSURE LIMIT VALUES
1.8.2	ACCEPTABLE RESIDUES LEVELS
1.8.3	WATER POLLUTION
1.8.4	MAJOR ACCIDENT HAZARDS
1.8.5	AIR POLLUTION
1.8.6	LISTINGS E.G. CHEMICAL INVENTORIES
1.9.1	DEGRADATION/TRANSFORMATION PRODUCTS
1.5.1	DEGLADATION THAT CHINATION THOUSEN
1.9.2	COMPONENTS
1.10	SOURCE OF EXPOSURE
1.11	ADDITIONAL DEMADICS
1.11	ADDITIONAL REMARKS
1.12	LAST LITERATURE SEARCH
1.13	REVIEWS

ld 92-94-4 **Date** 23.07.2003

# 2.1 MELTING POINT

**Value** : =  $210.1 - {}^{\circ}\text{C}$ 

Sublimation

Method : other: not reported

Year :

GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : SRC PhysProp Database.

Test substance : p-Terphenyl [CAS No. 92-94-4]

Reliability : (2) valid with restrictions

19.06.2003 (1)

## 2.2 BOILING POINT

Value :  $= 376 - ^{\circ}C$  at

Decomposition

Method : other: not reported

Year

GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : CRC Handbook; SRC PhysProp Database.

**Test substance** : p-Terphenyl [CAS No. 92-94-4] **Reliability** : (2) valid with restrictions

19.06.2003 (2) (1)

### 2.3 DENSITY

# 2.3.1 GRANULOMETRY

# 2.4 VAPOUR PRESSURE

**Value** : = .000000456 - hPa at 25 °C

Decomposition

**Method** : other (calculated)

Year :

GLP : no Test substance : other TS

Remark : Reported as 3.42 x 10e-7 mm Hg @ 25 deg. C.

Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : Neely and Blau. 1985.

**Test substance** : p-Terphenyl [CAS No. 92-94-4] **Reliability** : (2) valid with restrictions

19.06.2003 (3)

ld 92-94-4 **Date** 23.07.2003

### 2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water Log pow : = 6.03 - at °C

pH value : -

Method : other (measured): not reported

Year

GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : Sangster. 1993

**Test substance** : p-Terphenyl [CAS No. 92-94-4] **Reliability** : (2) valid with restrictions

19.06.2003 (4)

Partition coefficient : octanol-water Log pow : = 5.52 - at °C

pH value : -

Method : other (calculated): atom/fragment contribution method

Year :

GLP : no Test substance : other TS

Method : Individual atom/fragment contribution (AFC) values were determined for

130 simple chemical substructures. Another 235 correction factors were determined for various substructure orientations. The partition coefficient (log P) of a compound is estimated by summing all AFC values and

correction factors for a given chemical structure.

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : Meylan and Howard. 1995.
Test substance : p-Terphenyl [CAS No. 92-94-4]
Reliability : (2) valid with restrictions

19.06.2003 (5)

## 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water

**Value** : = .0018 - mg/l at 25 °C

pH value : -

concentration : at °C

Temperature effects

Examine different pol.

**pKa** : at 25 °C

**Description** : insoluble (< 0.1 mg/L)

Stable

Deg. product

Method : other: measured, method not reported

Year

GLP : no data
Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Source : Yalkowsky and Dannenfelser. 1992
Test substance : p-Terphenyl [CAS No. 92-94-4]

**Reliability** : (2) valid with restrictions

2.12 DISSOCIATION CONSTANT

ld 92-94-4 **Date** 23.07.2003

19.06.2003 (6)Solubility in : Water Value .055 - at 25 °C pH value concentration at °C Temperature effects Examine different pol. рKа at 25 °C Description **Stable** Deg. product Method other Year 1983 GLP no Test substance other TS Method Estimation of aqueous solubility was based on plotting the aqueous solubility vs the corrected retention time for calibration compounds. The estimation fit the following equation: log (RT)=-0.1946 log (uS)+1.091 with a linear correlation coefficient = 0.995, where RT=corrected retention time using reverse phase liquid chromatography and uS-aqueous solubility in u moles/L. A parallel estimation of water solubility used the method of Yalkowsky and Valvani (J.Chem. Eng. Data 24:127, 1979) which provided a correlation between aqueous solubility and octanol/water partition coefficient development. Remark Supplemental information provided on one isomeric component of Mixed Terphenyls [CAS 26140-60-3] Result Estimation of the aqueous solubility using the Calibration Curve method was 0.055 ppm while estimation of correlation with the Kow derived an estimate of 0.023 ppm. Test substance : p-Terphenyl Reliability (2) valid with restrictions 19.06.2003 (7)2.6.2 SURFACE TENSION 2.7 **FLASH POINT** 2.8 **AUTO FLAMMABILITY FLAMMABILITY** 2.9 **EXPLOSIVE PROPERTIES** 2.11 **OXIDIZING PROPERTIES** 

ld 92-94-4 **Date** 23.07.2003

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

ld 92-94-4 **Date** 23.07.2003

#### 3.1.1 PHOTODEGRADATION

Type : water
Light source : Sun light
Light spectrum : - nm

**Relative intensity** : - based on intensity of sunlight

Deg. product

**Method** : other (measured)

Year : 1983 GLP : no Test substance : other TS

Method : A 10 ppm solution of p-terphenyl was prepared in a 50:50 mixture of

deionized water and acetonitrile. The solutions were then poured into a series of quartz tubes which were placed in sunlight. Duplicate tubes were prepared but wrapped in aluminum foil to serve as a dark control. One light-exposed and one dark-control sample were analyzed on days 0, 1, 3, 7, 14 and 29. Weather conditions were generally sunny with daytime temp. reaching 90-95 deg. F. throughout the study. Sample preparation consisted of decanting 5 ml of the solution into a 15 ml centrifuge tube to which was added 3 g of NaCl to saturate the solution and separate acetonitrile from water. Isooctane (5 ml) was pipetted into the centrifuge tube and the mixture shaken vigorously for 2 min. One ml of isooctane was withdrawn and added to a GC autosampler vial. Anthracene was added as an internal standard. Extracts were analyzed by capillary GC using a flame ionization detector. Triplicate extracts were analyzed at 10 ppm and a

single extraction at 2 ppm.

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

**Result**: No significant decrease (<10%) in concentration was observed after 29

days of sunlight exposure. The %age of test material remaining (in parentheses) after days of exposure in sunlight/dark control were within experimental error. They were: day 0 (100%), day 1 (62/93%), day 3 (107/111%), day 7 (93/97%), day 14 (108/115%) and day 29 (90/101%). The absorbance of a 10 ppm acetonitrile:water (50:50) solution of p-

Terphenyl at 290 nm was 1.18/cm pathlength.

**Test substance**: Para-Terphenyl from Aldrich Chemical; purity unspecified.

**Reliability** : (2) valid with restrictions

19.06.2003 (8)

Type : other Light source :

**Light spectrum** : - nm

Relative intensity : - based on intensity of sunlight

Deg. product

Method : other (calculated): AOPWIN v1.90

Year :

GLP : no Test substance : other TS

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Vapor phase p -terphenyl is susceptible to reaction with photochemically produced hydroxyl (OH) radicals. The 2nd order rate constant for reaction with hydroxyl radicals was calculated as 9.1946E-12 cm3/(molecule\*sec). Based on 1.5E6 OH molecules/cm3 and assuming 12 hours of sunlight per

day, the estimated photo-oxidation half-life is 27.9 hours.

**Test substance** : p-Terphenyl [CAS No. 92-94-4]

**Reliability** : (2) valid with restrictions

ld 92-94-4 **Date** 23.07.2003

19.06.2003 (9)

### 3.1.2 STABILITY IN WATER

**Remark**: The test substance (p-Terphenyl) is not susceptible to hydrolysis.

13.05.2003

## 3.1.3 STABILITY IN SOIL

## 3.2.1 MONITORING DATA

## 3.2.2 FIELD STUDIES

## 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III

Media: other: air-water-soil-sedimentAir: 1.06 % (Fugacity Model Level I)Water: 11.7 % (Fugacity Model Level I)Soil: 45.3 % (Fugacity Model Level I)Biota: % (Fugacity Model Level II/III)Soil: 41.9 % (Fugacity Model Level II/III)

Method : other Year : 2003

Method : Used EPIWIN (Syracuse Research Corp., Syracuse, NY). The following

physical properties of p-terphenyl were used as model input parameters: water solubility = 0.0018 mg/L; vapor pressure of 3.42E-7 mm Hg; log Kow = 5.52; melting point = 210.1 deg. C. All property values were from this

Robust Summary.

**Remark** : Air: half life = 27.9 hr; emissions = 1000 kg/hr

Water: half life = 900 hr; emissions = 1000 kg/hr Soil: half life = 900 hr; emissions = 1000 kg/hr Sediment: half life = 3600 hr; emissions = 0 kg/hr

Persistence Time: 986 hr

Conclusion : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

**Reliability** : (2) valid with restrictions

19.06.2003

# 3.3.2 DISTRIBUTION

# 3.4 MODE OF DEGRADATION IN ACTUAL USE

# 3.5 BIODEGRADATION

Type : aerobic

ld 92-94-4 **Date** 23.07.2003

**Inoculum** : domestic sewage

**Concentration** : 20 mg/l related to Test substance

10 mg/l related to Test substance

Contact time : 42 day(s)

**Degradation** :  $0 - (\pm) \%$  after 42 day(s)

**Result**: under test conditions no biodegradation observed

Deg. product

**Method** : other: 42-day shake flask ultimate biodegradation

Year : 1991 GLP : yes Test substance : other TS

Method : Two test concentratons, 10 and 20 mg/L nominal, standard BOD medium

enhanced with 2 times normal amount of phosphate buffer, 4 times normal amount of FeCL3, and 40 mg (NH4)2SO4 per liter purified water; two liter triplicate flasks fitted with bar ium hydroxide solutions to catch CO2, sodium benzoate positive control. HgCL2-treated sterile control, inocula from acclimated solution prepared using 8-week SCAS procedure: activated mixed liquor plus raw filtered sewage, 1500 mL in glass vessels, stirred, aerated, suspended solids of 2500 to 5000 mg/L, 24-h cycle at end of which it was settled for 30 min, 1L decanted, 1L raw sewage added containing test substance at 1 mg/cycle via acetone. Initial bacterial count in test vessels inoculated with SCAS preparation was 6.1E+5 CFU/mL. At final day, residue analyzed using RP-HPLC-UV for remaining test material. Test vessels were incubated at 27 +/- 2 deg. C. in the dark on a rotary

shaker.

**Remark** : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Result : For the positive control, ~ 100 % thCO2 formed; for nominal 10 mg/L test

substance, 9% thCO2 formed; for 20 mg/L test material, 8% thCO2 formed. Analysis of day 42 residue showed that 81% and 78% remained, respectively, in tests using 10 and 20 mg/L test material. For the sterile control, 82% remained. NO volatile losses were reported. It was concluded that no appreciable degradation had occurred with the test substance.

**Test substance**: p-Terphenyl made up of 97.9% para, 1.7% meta- and 0.3% ortho-

Tamba and base up of 97.9% para, 1.7% meta- and 0.3% of the

Terphenyl isomer.

**Reliability** : (1) valid without restriction

13.05.2003 (10)

Type : aerobic Inoculum : other

**Concentration** : 20 mg/l related to Test substance

related to

Contact time : 55 day(s)

**Degradation** : =  $10 - (\pm 14)$  % after 55 day(s)

Result

Deg. product

Method : other
Year : 1983
GLP : no

**Test substance**: other TS

Method : Ultimate biodegradaton screening study using a shake flask carbon dioxide

procedure carried out over a 55-day period. Testing used a commercially available inoculum purported to be specifically adapted to hydrocarbons. The test material was exposed to a microbial population with a plate count of 1.3x10E8 colony-forming units/ml in an aqueous inorganic salts medium.

The BOD medium employed contained twice the standard level of phosphate buffer, four times the level of ferric chloride, the standard

amount of calcium chloride and magnesium sulfate and 40 mg (NH4)2 SO4 per liter of water. One L of medium was charged to a 2-L Erlenmeyer flask and sparged with 70% oxygen in nitrogen.A 10 mL aliquot of settled supernatant from the plending operation for medium preparation was

ld 92-94-4 **Date** 23.07.2003

supernatant from the blending operation for medium preparation was added to each test flask as the inoculum. After inoculum addition, 20 mg test chemical was added and triplicate flasks prepared. Each flask contained a reservoir holding barium hydroxide for capture and quantification of CO2 level. After sealing all flasks were agitated on a rotary shaker in the dark at ambient temperature until analyzed after 55 days on test. Analysis of the barium hydroxide solutions was performed using a Fisher Automated Titration system. The per cent carbon was calculated from molecular parameters. Glucose served as the reference chemical to verify methodology.

: Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Result : Following 55 days of exposure, a mean (3 reps) level of 10% (SD = 14)

with range of 0-26% CO2 evolution was achieved.

**Test substance** : Sample of p -Terphenyl obtained from Aldrich, with confirmed GC purity of

>95%.

**Reliability** : (2) valid with restrictions

09.07.2003 (11)

Type : aerobic

**Inoculum** : other:Mississippi River water

Contact time

Remark

**Degradation** :  $0 - (\pm) \%$  after 42 day(s)

**Result**: under test conditions no biodegradation observed

Deg. product :

Method : other: River Die Away Test

Year : 1983 GLP : no Test substance : other TS

Method : Samples of Mississippi River water (suspended solids= 51 mg/L; pH =

8.25; micorbial colonies/ml = 5.5x10E4), were allowed to settle for 2 days and then decanted through glass wool. Thereafter, 500 ml aliquots were placed in glass testing vessels. Each test jar was spiked with 50 ppb test material in methylene chloride, the jars sealed and stored at ambient temperature in the dark until sampled. One jar of test material and 1 jar of sterilized control water were sampled on test days 0, 1, 3, 7, 16, and 28. Bottles were extracted 3x with methylene chloride, the solvent condensed and analyzed using GC/FID. Analytical methodology had been verified for accuracy prior to study start. A second trial was conducted with another sample of Mississippi River water whereby each of the three Terphenyl isomers, ortho, meta and para, were added as a mixture at a rate of 20 ppb each. Similar procedures were followed for incubation and analysis, with one exception, this study was extended to 42 days for the final analysis.

**Remark**: Supplemental information which supports the conclusion that p-Terphenyl

is resistent to biological degradation in the environment.

Result : Even after a long (42-day) acclimation period, no appreciable

biodegradation occurred with p-Terphenyl in either Trial.

**Test substance** : para-Terphenyl, obtained from the Monsanto Procurement Laboratory, with

GC-confirmed purity > 95%. Samples of the other two Terphenyl isomers

used in the Mixture trial also were verified as > 95% pure.

**Reliability** : (2) valid with restrictions

03.06.2003 (12)

# 3.6 BOD5, COD OR BOD5/COD RATIO

### 3.7 BIOACCUMULATION

ld 92-94-4 **Date** 23.07.2003

3.8 ADDITIONAL REMARKS

4. Ecotoxicity ld 92-94-4

Pate 23.07.2003

#### 4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type

 Species
 : other: fish

 Exposure period
 : 96 hour(s)

 Unit
 : mg/l

 LC50
 : = .028

**Method** : other: calculated (EcoSAR)

Year

GLP : no Test substance : other TS

Remark : An acute fish 96-h LC50 was calculated using ECOSAR, from the USEPA.

The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within

ECOSAR.

**Test substance** : p-Terphenyl [CAS No. 92-94-4]

**Conclusion** : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

13.05.2003 (13)

# 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static

Species : Daphnia magna (Crustacea)

**Exposure period** 48 hour(s) Unit mg/l **NOEC** > 5.5 -EC50 > 5.5 -**Analytical monitoring** Method : other Year 1983 : **GLP** : yes : other TS Test substance

Remark

Method : Used EPA method (1975) 660/3-75-009 Committee on Methods for Acute

Toxicity Tests with Fish, Macroinvertebrates and Amphibians. Ten <24-h old D. magna Straus were selected from an in-house colony and tested at 20 +/-1 deg. C in a series of three replicates per test concentration. Test concentrations were 0.344, 0.688, 1.375, 2.75 and 5.5 mg/L, plus clean water and solvent (dimethylformamide) controls. Tests were conducted in capped test vessels to preclude volatilization and used well water from St. Peters, Mo. Photoperiod employed was unspecified. Concentrations were not meas ured. Daphnids were not fed. Tests were conducted in 8-oz. glass beakers containing 200 mL of solution. Water quality was measured for Dissolved Oxygen, pH, alkalinity, water hardness, and temperature. No significant change were observed in any parameter measured.

: Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

Result : 48-h EC50 > 5.5 mg/L. NOEC > 5.5 mg/L. % immobility (in parenthesis)

seen after 24-h: control (0), solvent control (0), 0.344 mg/L (0), 0.688 mg/L (0), 1.375 mg/L (0), 2.75 mg/L (0), and 5.5 mg/L (3); and at 48-hr: control (0), solvent control (0), 0.344 mg/L (0), 0.688 mg/L (0), 1.375 mg/L (0), 2.75 mg/L (3), and 5.5 mg/L (3). pH ranged from 7.8-8.0; DO ranged from 8.0-8.7; alkalinity ranged from 256-262 mg/L CaCO3; hardness ranged from 230-244 mg/L CaCO3. Visual inspection of all test containers indicated that the water solubility level of this chemical was exceeded. In a range-find study, at nominal test concentrations (0.005, 0.01, 0.05, and 0.1

4. Ecotoxicity ld 92-94-4

Pate 23.07.2003

range-find study, at nominal test concentrations (0.005, 0.01, 0.05, and 0.1 mg/L) below visual indications of insolubility, no more than 1 % immobility

was observed.

**Test substance** : Analytical grade sample p-Terphenyl; purity unknown.

**Reliability** : (2) valid with restrictions

23.07.2003 (14)

Type

Species : Daphnia sp. (Crustacea)

 Exposure period
 : 48 hour(s)

 Unit
 : mg/l

 LC50
 : = .039 

Method : other: calculated (EcoSAR)

Year :

GLP : no Test substance : other TS

Remark : An acute Daphnia 48-h LC50 was calculated using ECOSAR, from the

USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES

notations within ECOSAR.

**Test substance** : p-Terphenyl [CAS No. 92-94-4]

**Conclusion** : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

13.05.2003 (13)

### 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

**Species** : other algae: green algae

Endpoint

 Exposure period
 : 96 hour(s)

 Unit
 : mg/l

 LC50
 : = .031 

Method : other: calculated (EcoSAR)

Year

GLP : no Test substance : other TS

Remark : An acute green algal 96-h LC50 was calculated using ECOSAR, from the

USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES

notations within ECOSAR.

**Test substance** : p-Terphenyl [CAS No. 92-94-4]

**Conclusion** : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]

13.05.2003 (13)

# 4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

# 4.5.1 CHRONIC TOXICITY TO FISH

# 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

# 4. Ecotoxicity

4.9 ADDITIONAL REMARKS

4.6.1	TOXICITY TO SEDIMENT DWELLING ORGANISMS
162	TOXICITY TO TERRESTRIAL PLANTS
4.0.2	TOAIGHT TO TERRESTRIAL FEARTS
4.6.3	TOXICITY TO SOIL DWELLING ORGANISMS
4.6.4	TOX. TO OTHER NON MAMM, TERR. SPECIES
4.0.4	TOA. TO OTHER NON IMAIVIIVI. TERR. SPECIES
4.7	BIOLOGICAL EFFECTS MONITORING
4.0	DISTRIBUTED AND MULTIPLE
4.8	BIOTRANSFORMATION AND KINETICS

5. Toxicity ld 92-94-4

Date 23.07.2003

### 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

### 5.1.1 ACUTE ORAL TOXICITY

Type : LD0

**Value** : > 10000 - mg/kg bw

Species : rat

Strain : Sprague-Dawley
Sex : male/female

Number of animals

Vehicle : other

Doses : 500-10000 mg/kg
Method : other (calculated)

Year : 1962 GLP : no Test substance : other TS

Method : Method used consistent with OECD 401, but conducted prior to its

codification. Groups of 5 male and female SD rats were administered test material in logarithmetically spaced dosages between 500 and 10,000 mg/kg. Each dosage was given once by gavage as a 20% suspension in corn oil. Animals were observed for 14 days after which they were necropsied. After determination of the LD0 additional groups of 5 rats were administered the test article in a similar fashion at dosages of 2000, 4000 and 10000 mg/kg and observed for up to 14 days. During this period, checks on food consumption and body weight were made and obervation of clinical signs of toxicity recorded. Lives and kidney weights (and

of clinical signs of toxicity recorded. Liver and kidney weights (and corresponding organ:body weight ratios) were calculated. Necopsies were performed and histopathological examinations were conducted on the following organs: heart, liver, lung, adrenals, kidneys and spleen.

Remark : Supplemental information provided on one isomeric component of Mixed

Terphenyls [CAS 26140-60-3]. Study adequate to provide corroborative

information in assessment of mixed terphenyls.

Result : LD0 > 10,000 mg/kg Consistent signs of toxicity were observe d in most

animals, including rough coat and diarrhea. However, no deaths occurred at 10,000 mg/kg (highest dose tested). No effects noted in body weights or

necropsy or histopathology, with the exception of possible liver

regeneration.

**Test substance** : Reagent grade para-terphenyl, with purity verified but unspecified.

**Reliability** : (2) valid with restrictions

13.05.2003 (15)

## 5.1.2 ACUTE INHALATION TOXICITY

## 5.1.3 ACUTE DERMAL TOXICITY

# 5.1.4 ACUTE TOXICITY, OTHER ROUTES

# 5.2.1 SKIN IRRITATION

5. Toxicity ld 92-94-4

Pate 23.07.2003

### 5.2.2 EYE IRRITATION

### 5.3 SENSITIZATION

## 5.4 REPEATED DOSE TOXICITY

Type : Sub-acute
Species : rat
Sex : no data

Strain : Sprague-Dawley

Route of admin. : oral feed Exposure period : 30 days Frequency of treatm. : daily Post exposure period : none

**Doses** : 500, 250 and 100 mg/kg body weight

Control group : yes

**NOAEL** : = 250 - mg/kg bw

Method: otherYear: 1962GLP: noTest substance: other TS

Method : Groups of 5 SD rats (sex unspecified) were fed inhouse diet admixed with

either 100, 250 or 500 mg/kg/body wt. test material for 30 consecutive days. Water was administered ad libitum. All rats underwent gross necropsy at the end of the study and liver and kidney weights recorded. Body weights were measured on test days 11, 21 and 28. Heart, liver, lungs, kidneys, adrenals and spleen were examined microscopically at all

test levels

Result : 250 mg/kg - Overall NOEL. At 500 mg/kg/d - A significant reduction in

body weight was observed at the end of the study. No treatment-related effects were noted in liver or kidney weights/weight ratios or after

histopathological examination of organs.

Test substance : Reagent grade para-terphenyl purchased from Eastman Chemical and

confirmed for purity but unspecified.

**Reliability** : (2) valid with restrictions

Provided as Supplemental information; this study provides additional subacute information of some reliance on one of the terphenyl isomers

found in Mixed Terphenyls.

29.04.2003 (15)

Type : Sub-acute
Species : rat
Sex : male
Strain : Wistar
Route of admin. : oral feed
Exposure period : 14 days
Frequency of treatm. : daily
Post exposure period : none

**Doses** : 0.2 % in the diet (2000 ppm)

Control group : yes
LOAEL : = .2 - %

Method : other

Year : 1974

GLP : no

Test substance : other TS

5. Toxicity ld 92-94-4

Date 23.07.2003

**Method** : An unspecified number of young, adult male Wistar rats were administered

commercial diet containing 0.2% (2000 ppm) test material in corn oil (test material dissolved in diethyl ether) for 14 consecutive days. Food and water were provided ad libitum and recorded daily. Organs (liver, kidney, spleen, adrenal) were weighed at necrospy after 2 weeks on test. Blood was taken via heart puncture at the end of the study to assess plasma and

liver cholesterol. Unspecified statistical methods used with p<0.05.

: After 14 days of testing a significant increase (118%) in plasma cholesterol

level was observed. No other effects noted at this test level.

**Test substance**: Para-Terphenyl obtained from Wako Pure Chemical Co., Tokyo.

**Reliability** : (4) not assignable

Provided as Supplemental information.

13.05.2003 (16)

## 5.5 GENETIC TOXICITY 'IN VITRO'

# 5.6 GENETIC TOXICITY 'IN VIVO'

# 5.7 CARCINOGENICITY

Result

## 5.8.1 TOXICITY TO FERTILITY

### 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

# 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Type : other
In vitro/in vivo : In vitro
Species : mouse
Sex : male/female
Strain : other
Route of admin. : other

**Exposure period** : 20-24 hr incubation

Frequency of treatm. : once

Duration of test

**Doses** : 0, 0.1, 1, and 10 ug/mL

Control group : yes

Result : Increased number of abnormal embryos and degenerative oocytes at and

above 1 ug/mL.

Method: otherYear: 1994GLP: no dataTest substance: other TS

Method : Used the mouse in vitro fertilization (IVF) technique to measure effects on

fertilization and early embryo development. Male and female mice from inhouse-bred strain B6D2F1 young adults were used. Food and water were provided ad libitum while light cycle and temperature were controled. Female mice were superovulated by IP injection of 10 IU of serum gonadotropin followed by 10 IU human chorionic gonadotropin (HCG). 12-15 hrs after addition of HCG, sperm was collected from the cauda

epididymides from adult male mice. After verification of sperm viability and motility, oocytes were recovered from superovulated mice and exposed to

18/24

ld 92-94-4 5. Toxicity Date 23.07.2003

> motility, oocytes were recovered from superovulated mice and exposed to 2-3 million sperm in an incubation medium containing test material for 20-24 hrs. Test substance was suspended in BMOC-3 culture medium with minimal alcohol (0.01%) and then mixed with medium to attain dosages of 0.1, 1 or 10 ug/mL test substance. Each culture dish containing test material, sperm and oocytes was scored for fertilized or degenerative oocytes and abnormal embryos. Fertilization was considered to have occurred in the presence of 1 cell with 2 pronuclei, 2 cells with 1 polar body or a 2-celled embryo. Three-to-5 trials were conducted per test concentration. Mean scores were statistically evaluated using Chi Square and Bonferroni Chi Square Contingency Tables with p<0.05.

Remark Supplemental information; study inadequate to support this HPV endpoint. Result

No treatment-related effects were observed at 0.1 ug/mL. An increase in the number of embryos and degenerative oocytes was observed at 1 and 10 ug/mL No overall statistically significant decrease in IVF was reported although there was a small decrease in IVF at 10 ug/mL vs control.

**Test substance** Purchased from AccuStandard, Inc. CT and verified by GC-FID as 99%

pure para-Terphenyl

Reliability (3) invalid

19.06.2003 (17)

#### 5.9 SPECIFIC INVESTIGATIONS

## 5.10 EXPOSURE EXPERIENCE

# 5.11 ADDITIONAL REMARKS

# 6. Analyt. Meth. for Detection and Identification

- 6.1 ANALYTICAL METHODS
- 6.2 DETECTION AND IDENTIFICATION

# 7. Eff. Against Target Org. and Intended Uses

7.1	FUNCTION
7.2	EFFECTS ON ORGANISMS TO BE CONTROLLED
1.2	EFFECTS ON ORGANISIVE TO BE CONTROLLED
7.3	ORGANISMS TO BE PROTECTED
7.4	USER
7.5	RESISTANCE
7.3	REJIJ I ANCE

# 8. Meas. Nec. to Prot. Man, Animals, Environment

8.1	METHODS HANDLING AND STORING
8.2	FIRE GUIDANCE
8.3	EMERGENCY MEASURES
8.4	POSSIB. OF RENDERING SUBST. HARMLESS
8.5	WASTE MANAGEMENT
8.6	SIDE-EFFECTS DETECTION
0.0	
8.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
0.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
88	REACTIVITY TOWARDS CONTAINER MATERIAL

# 9. References Id 92-94-4 Date 23.07.2003

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Biphenyls and Perchlorinated Terphenyls on In Vitro Fertilization in the Mouse. Arch

Environ Contam Toxicol. 26: 208-211.

# 10. Summary and Evaluation

ld 92-94-4 **Date** 23.07.2003

10.1	<b>FND</b>	<b>POINT</b>	·SL	JMM	ARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

# IUCLID

# **Data Set**

Existing Chemical : ID: 29036-02-0 CAS No. : 29036-02-0 Common name : Quaterphenyl EINECS Name : Quaterphenyl Molecular Formula : C24H18 EC No. : 249-380-1

Producer related part

Company : Solutia Inc.
Creation date : 17.03.2003

Substance related part

Company : Solutia Inc. Creation date : 17.03.2003

Status : Memo :

Printing date : 23.07.2003

Revision date

Date of last update : 23.07.2003

Number of pages : 20

**Chapter (profile)** : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 **Reliability (profile)** : Reliability: without reliability, 1, 2, 3, 4

Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),

Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

# 1. General Information

1.0.1	APPLICANT AND COMPANY INFORMATION
1.0.2	LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR
1.0.3	IDENTITY OF RECIPIENTS
1.0.4	DETAILS ON CATEGORY/TEMPLATE
1.1.0	SUBSTANCE IDENTIFICATION
1.1.1	GENERAL SUBSTANCE INFORMATION
1.1.2	SPECTRA
1.2	SYNONYMS AND TRADENAMES
1.3	IMPURITIES
1.4	ADDITIVES
1.5	TOTAL QUANTITY
1.6.1	LABELLING
1.6.2	CLASSIFICATION
1.6.3	PACKAGING
1.7	USE PATTERN
1.7.1	DETAILED USE PATTERN
1.7.2	METHODS OF MANUFACTURE

# 1. General Information

1.8	REGULATORY MEASURES
1.8.1	OCCUPATIONAL EXPOSURE LIMIT VALUES
400	ACCEPTABLE DECIDIFICAL EVELO
1.8.2	ACCEPTABLE RESIDUES LEVELS
1.8.3	WATER POLLUTION
1.8.4	MAJOR ACCIDENT HAZARDS
1.8.5	AIR POLLUTION
1.8.6	LISTINGS E.G. CHEMICAL INVENTORIES
1.9.1	DEGRADATION/TRANSFORMATION PRODUCTS
1.9.2	COMPONENTS
1.10	SOURCE OF EXPOSURE
1.11	ADDITIONAL REMARKS
4.40	LACTURED ATURE OF A DOLL
1.12	LAST LITERATURE SEARCH
1.13	REVIEWS

ld 29036-02-0 **Date** 23.07.2003

# 2.1 MELTING POINT

**Value** : 160 - 200 °C

Sublimation

Method : other: Internal analysis

**Year** : 1990

GLP

Test substance : other TS

**Test substance** : Santotar 9 consisting of a 100% polyphenyl mixture made up of 95%

Quaterphenyls and Higher Polyphenyls and < 1% Mixed Terphenyls.

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

09.07.2003

Value : = 184.1 °C

Sublimation

Method : other: calculated (MPBPWIN v1.40)

Year :

GLP : no Test substance : other TS

Source : EPIWIN

**Test substance** : Quaterphenyl [CAS No. 29036-02-0]

**Reliability** : (2) valid with restrictions

09.07.2003 (2)

# 2.2 BOILING POINT

**Value** : > 420 °C at

Decomposition

Method : other: Internal analysis

**Year** : 1990

GLP

Test substance : other TS

**Test substance** : Santotar 9 consisting of a 100% polyphenyl mixture made up of 95%

Quaterphenyls and Higher Polyphenyls and < 1% Mixed Terphenyls.

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

23.07.2003 (3)

Value : = 481.2 °C at

Decomposition :

Method : other: calculated (MPBPWIN v1.40)

Year :

GLP : no Test substance : other TS

Source : EPIWIN

Test substance : Quaterphenyl [CAS No. 29036-02-0]

**Reliability** : (2) valid with restrictions

09.07.2003 (2)

### 2.3 DENSITY

ld 29036-02-0 **Date** 23.07.2003

# 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

**Value** : = .00000000237 hPa at 25 °C

Decomposition

Method : other (calculated): MPBPWIN v1.40

Year

GLP : no Test substance : other TS

Remark : Reported as 1.78e-9 mm Hg @ 25 deg. C.

Source : EPIWIN

Test substance : Quaterphenyl [CAS No. 29036-02-0]

**Reliability** : (2) valid with restrictions **Flag** : Critical study for SIDS endpoint

09.07.2003 (2)

## 2.5 PARTITION COEFFICIENT

**Partition coefficient** : octanol-water **Log pow** : = 7.28 at °C

pH value

Method : other (calculated): KOWWIN v1.66

Year

GLP : no Test substance : other TS

Source : EPIWIN

**Test substance**: Quaterphenyl [CAS No. 29036-02-0]

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

19.06.2003 (4)

# 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water

**Value** : .002 at 25 °C

pH value

concentration : at °C

Temperature effects

Examine different pol.

**pKa** : at 25 °C

Description Stable

Deg. product

Method : other: Internal analysis

Year : 1990
GLP : yes
Test substance : other TS

Method : Used two water samples (tap and well water) and analyzed via LC

methodology with confirmed detection limit to 0.000102 mg/L.

**Test substance** : Santotar 9 consisting of a 100% polyphenyl mixture made up of 95%

Quaterphenyls and Higher Polyphenyls and < 1% Mixed Terphenyls.

ld 29036-02-0 **Date** 23.07.2003

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

09.07.2003 (5)

Solubility in : Water

**Value** : = .00677 mg/l at 25 °C

pH value

concentration : at °C

Temperature effects

Examine different pol.

**pKa** : at 25 °C

**Description** : insoluble (< 0.1 mg/L)

Stable .

Deg. product

Method : other: calculated (WSKOW v1.37)

Year :

GLP : no Test substance : other TS

Source : EPIWIN

**Test substance**: Quaterphenyl [CAS No. 29036-02-0]

**Reliability** : (2) valid with restrictions

09.07.2003 (6)

# 2.6.2 SURFACE TENSION

# 2.7 FLASH POINT

# 2.8 AUTO FLAMMABILITY

## 2.9 FLAMMABILITY

# 2.10 EXPLOSIVE PROPERTIES

# 2.11 OXIDIZING PROPERTIES

# 2.12 DISSOCIATION CONSTANT

# 2.13 VISCOSITY

# 2.14 ADDITIONAL REMARKS

ld 29036-02-0 **Date** 23.07.2003

### 3.1.1 PHOTODEGRADATION

Type : other Light source :

**Light spectrum** : nm

**Relative intensity**: based on intensity of sunlight

Deg. product :

Method : other (calculated): AOPWIN v1.90

Year : 2002 GLP : no Test substance : other TS

**Remark**: Vapor phase quaterphenyls are susceptible to reaction with

photochemically produced hydroxyl (OH) radicals. The 2nd order rate constant for reaction with hydroxyl radicals was calculated as 18.544E-12 cm3/(molecule\*sec). Based on 1.5E6 OH molecules/cm3 and assuming 12 hours of sunlight per day, the estimated photo-oxidation half-life is 13.8

hours.

Source : EPIWIN

**Test substance**: Quaterphenyl [CAS No. 29036-02-0]

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

23.07.2003 (7)

# 3.1.2 STABILITY IN WATER

**Remark**: The test substance (Quaterphenyl) is not susceptible to hydrolysis. It has

only 4-membered aromatic rings associated with its structure, which are listed in Lyman in Table 7.1- Types of Organic Functional Groups That Are Generally Resistant to Hydrolysis. Lyman, WJ, Reehl, WF and Rosenblatt,

DH. 1990. Handbook of Chemical Property Estimation Methods.

Environmental Behaviour of Organic Compounds. American Chemical

Society, Washington, DC.

02.06.2003

## 3.1.3 STABILITY IN SOIL

# 3.2.1 MONITORING DATA

### 3.2.2 FIELD STUDIES

# 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III

Media

Air : .218 % (Fugacity Model Level I)

Water : 3.47 % (Fugacity Model Level I)

Soil : 32.3 % (Fugacity Model Level I)

Biota : % (Fugacity Model Level II/III)

Soil : 64.1 % (Fugacity Model Level II/III)

ld 29036-02-0 **Date** 23.07.2003

Method: otherYear: 2002

Method : Used EPIWIN (2002), Syracuse Research Corp, Syracuse, NY. Physical

properties of quaterphenyl used as the model input parameters were water solubility of 0.00677 mg/L, vapor pressure of 1.78E-9 mm Hg, log Kow of 7.28, and melting point point of 184.1 deg. C. All property values were

taken from this IUCLID dossier.

**Remark**: Air: half-life = 13.8 hr, emissions = 1000 kg/hr

Water: half-life = 900 hr; emissions = 1000 kr/hr Soil: half-life = 900 hr, emissions = 1000 kg/hr. Sediment: half-life = 3600 hr, emissions = 0 kg/hr

Persistence Time - 1740

**Test substance**: Quaterphenyls [CAS no. 29036-02-0]

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

23.07.2003

## 3.3.2 DISTRIBUTION

## 3.4 MODE OF DEGRADATION IN ACTUAL USE

## 3.5 BIODEGRADATION

Type : aerobic Inoculum : other

**Concentration** : 20 mg/l related to Test substance

related to

Contact time : 55 day(s)

**Degradation** :  $= 7 (\pm 9) \%$  after 55 day(s)

Result : Deg. product :

 Method
 : other

 Year
 : 1983

 GLP
 : no

 Test substance
 : other TS

Method : Ultimate biodegradation screening study using a shake flask carbon

dioxide procedure carried out over a 55-day period. Testing used a commercially available inoculum purported to be specifically adapted to hydrocarbons. The test material was exposed to a microbial population with a plate count of 1.3x10E8 colony-forming units/ml in an aqueous inorganic salts medium. The BOD medium employed contained twice the standard level of phosphate buffer, four times the level of ferric chloride, the standard amount of calcium chloride and magnesium sulfate and 40 mg (NH4)2 SO4 per liter of water. One L of medium was charged to a 2-L Erlenmeyer flask and sparged with 70% oxygen in nitrogen. A 10 mL aliquot of settled supernatant from the blending operation for medium preparation was added to each test flask as the inoculum. After inoculum addition, 20 mg test chemical was added and triplicate flasks prepared. Each flask contained a reservoir holding barium hydroxide for capture and quantification of CO2 level. After sealing all flasks were agitated on a rotary shaker in the dark at ambient temperature until analyzed after 55 days on test. Analysis of the barium hydroxide solutions was performed using a Fisher Automated Titration system. The per cent carbon was calculated from molecular parameters. Glucose served as the reference chemical to

verify methodology.

8/20

ld 29036-02-0 **Date** 23.07.2003

verify methodology.

Result : Following 55 days of exposure, a mean (3 reps) level of 7% (SD=9) with a

range of 0-16% CO2 evolution was achieved.

**Test substance** : Sample of Quaterphenyl isomer with a verified (GC) purity of > 95% and

obtained from the Monsanto Chemical Procurement Laboratory.

**Reliability** : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

23.07.2003 (8)

Type : aerobic

Inoculum

Contact time

**Degradation** : 54 (±) % after 7.5 month

Result

Deg. product

**Method** : other: Soil microbial biodegradation

Year : 1988
GLP : no
Test substance : other TS

Method : Used a defined methodology to determine the degree of biodegradability

caused by soil microorganisms from two separate soil samples. Two concentrations of test material (50 ppm and 0.5 ppm) were prepared in methylene chloride. Two soil types, (1) Missouri Bottoms, a sandy soil with 0.5% organic carbon and a moisture content of 11.3% at 1/3 BAR and (2) Florida muck, a heavy loam containing 32.9% organic carbon and an 82% moisture content at 1/3 BAR. Soil samples containing test material were analyzed by HPLC after 0, 0.5, 1, 2, 4, 6, 8, 12, 15, and 32 weeks on study. A microtox screen was employed prior to study start to insure no bacterial toxicity would interfere with the subsequent test. Method of detection of test material was validated on both soils pres tudy. Soil samples were stabilized

prior to study start such that they contained a uniform level of microorganisms. Soil samples (25 gm) were placed in 125 ml jars and spiked with 250 ul of test solution containing the test material in solvent. Jars were capped and shaken, then lids removed and restirred manually. After being lightly recapped, the jars containing the test material and soil were incubated in the dark at 25 deg. C and 80% humidity until sampled. Three replicates of each treated group plus a control per time period per

soil type were used. Sterile controls and matrix blanks were also employed. Kinetic parameters were calculated from raw data.

**Remark**: Provided as Supplementary information.

Result : % Reduction Relative to Nominal Concentration after 32 Weeks on Test

Nominal Conc. % Red. Soil Type % Vs Sterile Soil T 1/2 (weeeks)

500 ppm 54 Mo. Bott. -35 28.9 0.5 ppm 50 Mo. Bott. - 32.0

500 ppm 42 Fla Muck 27 40.9 0.5 ppm 33 Fla Muck - 54.7

Quaterphenyl underwent little biological degradation upon introduction to either sandy or loam soil types containing soil bacteria. The degree of loss seen in the sandy soil was essentially the same as seen in the sterilized control. Thus, most of the loss observed in nonsterile soil was considered abiotic. Some biologically-mediated degradation was observed in the Fla. Muck soil.

**Test substance** : Sample labeled "Quaterphenyls"

**Reliability** : (2) valid with restrictions

19.06.2003 (9)

- 3.6 BOD5, COD OR BOD5/COD RATIO
- 3.7 BIOACCUMULATION
- 3.8 ADDITIONAL REMARKS

ld 29036-02-0 4. Ecotoxicity Date 23.07.2003

### ACUTE/PROLONGED TOXICITY TO FISH

Type

Species other: fish Exposure period 96 hour(s) Unit mg/l LC50 = .002

Method other: calculated (EcoSAR)

Year

**GLP** Test substance other TS

Remark : An acute fish 96-h LC50 was calculated using ECOSAR, from the USEPA.

> The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES notations within

ECOSAR.

Test substance : Quaterphenyl [CAS No. 29036-02-0]

13.05.2003 (10)

#### **ACUTE TOXICITY TO AQUATIC INVERTEBRATES** 4.2

Type flow through

**Species** Daphnia magna (Crustacea)

**Exposure period** 48 hour(s) Unit mg/l = .008 **NOEC** EC50 >= .069

**Analytical monitoring** 

Result

Method other: EPA 660/3-75-009, 560/6-82-002

Year 1993 GLP : yes Test substance other TS

Method : Ten <24-h old D. magna Straus were tested at 20 +/- 1 deg C. in a series

> of two replicates per test concentration. Nominal test concentrations were 0.006, 0.012, 0.025, 0.05, and 0.1 mg/L, plus clean water and solvent (dimethylformamide) control. A half-liter proportional diluter system was used to introduce TS. One liter glass beakers with notched drains covered with 50-mesh stainless steel screen were used as the test chamber. Tests were conducted using reconstituted water prepared to a total harness of 130 to 160 mg/L CaCO3. Concentrations were measured analytically. Daphnids were not fed during the test. Lighting was on a 16-h day: 8-h night cycle with 30 min. transition periods. Dissolved oxygen was

monitored to ensure the concentration did not fall below 2 mg/L before the

end of the test.

Water quality was measured for dissolved oxygen, pH and temperature and no significant changes were observed in any parameter during the test. Statistical analyses were performed according to USEPA procedures.

Mean measured concentrations of the TS were 0.004, 0.008, 0.016, 0.031

and 0.069 mg/L. Daphnids were observed to surface at the 0.016 mg/L level and above. All solutions were considered visually clear. Temperature ranged from 20-21 deg.C, pH ranged from 8.2-8.4, DO ranged from 7.4 to 8.0 mg/L, hardness ranged from 134 to 146 mg/L as CaCO3, alkalinity was 160 mg/L CaCO3. Immobilizations ranged betwen 0 and 10% across all concentrations and controls at both the 24-h and 48-h time points.

24-h EC50 = > 0.069 mg/L48-h EC50 = > 0.069 mg/L

11/20

ld 29036-02-0 4. Ecotoxicity Date 23.07.2003

48-h EC50 = > 0.069 mg/L

NOEC = 0.008 mg/L.

Test substance Santotar 9, a 100% polyphenyl mixture made up of 95% Quaterphenyls

and 5% Mixed Terphenyls.

Reliability (1) valid without restriction : Critical study for SIDS endpoint Flag

19.06.2003 (11)

Type

**Species** Daphnia sp. (Crustacea)

Exposure period 48 hour(s) Unit mg/l LC50 = .004

Method other: calculated (EcoSAR)

Year

GLP Test substance other TS

Remark : An acute Daphnia 48-h LC50 was calculated using ECOSAR, from the

USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES

notations within ECOSAR.

Test substance Quaterphenyl [CAS No. 29036-02-0]

Reliability (2) valid with restrictions

15.05.2003 (10)

#### TOXICITY TO AQUATIC PLANTS E.G. ALGAE 4.3

**Species** other algae: green algae

**Endpoint** 

**Exposure period** 96 hour(s) Unit mg/l LC50 =.003

Method other: calculated (EcoSAR)

Year

GLP Test substance

other TS

Remark : An acute green algal 96-h LC50 was calculated using ECOSAR, from the

> USEPA. The SAR for esters was used. The structure was determined from the CAS RN, as stored in the accompanying database of SMILES

notations within ECOSAR.

Test substance : Quaterphenyl [CAS No. 29036-02-0]

13.05.2003 (10)

# TOXICITY TO MICROORGANISMS E.G. BACTERIA

# 4.5.1 CHRONIC TOXICITY TO FISH

# 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

# 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

# 4. Ecotoxicity

4.6.2 TOXICITY TO TERRESTRIAL PLANTS	
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- 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS
- 4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES
- 4.7 BIOLOGICAL EFFECTS MONITORING
- 4.8 BIOTRANSFORMATION AND KINETICS
- 4.9 ADDITIONAL REMARKS

5. Toxicity ld 29036-02-0

Pate 23.07.2003

### 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

## 5.1.1 ACUTE ORAL TOXICITY

Type : LD50

**Value** : = 5650 - mg/kg bw

Species : rat

Strain : Sprague-Dawley
Sex : male/female

Number of animals : 20 Vehicle : other

**Doses** : 3980, 5010, 6310, and 7940 mg/kg

**Method** : other (calculated)

Year : 1974 GLP : no Test substance : other TS

**Method**: Groups of 5 mixed sex young adult rats were administered logarithmetically

spaced dosages of test material by single gavage dose. Each dosage was prepared as a 20% suspension in corn oil, after heating to 115 Deg. F. Observations for toxicity were made daily for 14 consecutive days. All animals underwent a necropsy. Food and water were provided ad libitum; humidity, temperature and light cycle were controled. Body weights were recorded on test days 0, 7 and 14. LD50 value and Cl were determined by

the method of Litchfield and Wilcoxon, 1949.

**Remark**: Study conducted according to OECD 401 design but with some limitations

(i.e., smaller sample size); however, results are sufficiently robust to

support this endpoint for HPV program.

**Result** : LD50 (95% CL) = 5,650 (5370-5930) mg/kg. Most deaths occurred within

4 days. No. dead/5 animals (in parenthesis) per test group: 1980 mg/kg (0/5), 5010 mg/kg (1/5), 6310 mg/kg (4/5), and 7940 mg/kg (5/5). Generalized signs of toxicity (data not available for individual animals) included weakness, reduced appetite and hypoactivity. Liver discoloration and acute gi inflammation were observed in decendents at necropy;

viscera of all survivors appeared normal at necropsy.

**Test substance**: Santowax Q, consisting of 95% Quaterphenyls and 5% Mixed Terphenyls.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

23.07.2003 (12)

# 5.1.2 ACUTE INHALATION TOXICITY

# 5.1.3 ACUTE DERMAL TOXICITY

# 5.1.4 ACUTE TOXICITY, OTHER ROUTES

# 5.2.1 SKIN IRRITATION

# 5.2.2 EYE IRRITATION

# 5. Toxicity ld 29036-02-0 Date 23.07.2003

5.3	SENSITIZATION
5.4	REPEATED DOSE TOXICITY
5.5	GENETIC TOXICITY 'IN VITRO'
5.6	GENETIC TOXICITY 'IN VIVO'
5.7	CARCINOGENICITY
5.8.1	TOXICITY TO FERTILITY
5.8.2	DEVELOPMENTAL TOXICITY/TERATOGENICITY
5.8.3	TOXICITY TO REPRODUCTION, OTHER STUDIES
0.0.0	1974911 19742 Reporter, emarker epise
5.9	SPECIFIC INVESTIGATIONS
0.0	
5.10	EXPOSURE EXPERIENCE
3.10	LAI OOOAL LAI LIALIACE
5.11	ADDITIONAL REMARKS
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# 6. Analyt. Meth. for Detection and Identification

- 6.1 ANALYTICAL METHODS
- 6.2 DETECTION AND IDENTIFICATION

# 7. Eff. Against Target Org. and Intended Uses

7.1	FUNCTION
7.2	EFFECTS ON ORGANISMS TO BE CONTROLLED
7.3	ORGANISMS TO BE PROTECTED
7.4	USER
7.5	RESISTANCE

# 8. Meas. Nec. to Prot. Man, Animals, Environment

8.1	METHODS HANDLING AND STORING
8.2	FIRE GUIDANCE
8.3	EMERGENCY MEASURES
8.4	POSSIB, OF RENDERING SUBST, HARMLESS
-	
8.5	WASTE MANAGEMENT
0.10	
8.6	SIDE-EFFECTS DETECTION
0.0	GDE ET EGTO DETEGTION
8.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
0.7	SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER
88	REACTIVITY TOWARDS CONTAINER MATERIAL
XX	REALTIVITY TOWARDS CONTAINER WATERIAL

9. References ld 29036-02-0
Date 23.07.2003

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# 10. Summary and Evaluation

ld 29036-02-0 **Date** 23.07.2003

10.1	<b>FND</b>	<b>POINT</b>	·SI	<b>JMM</b>	ARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT